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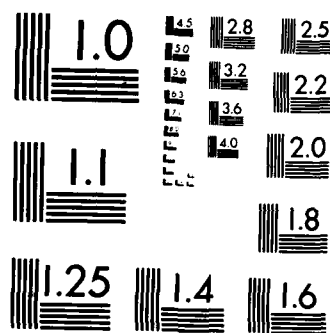


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by

H. T. Banks

and

P. L. Daniel

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LCDS Report #82-22

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ESTIMATION OF VARIABLE COEFFICIENTS IN  
PARABOLIC DISTRIBUTED SYSTEMS

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ESTIMATION OF VARIABLE COEFFICIENTS IN  
PARABOLIC DISTRIBUTED SYSTEMS

H. T. Banks and P. L. Daniel

ABSTRACT

We present techniques based on cubic spline approximations for estimating coefficients (e.g., diffusion, convective velocity, etc.) depending on time and the spatial variable in parabolic distributed systems such as those that arise in transport models. Convergence results and a summary of numerical performance of the resulting algorithms are given.



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## §1 Introduction

In this paper we present results on the problem of estimating variable (in space and time) coefficients in general parabolic models. Our efforts were motivated by consideration of fundamental transport equations (based on mass balance) such as

$$(1.1) \quad \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} (Vu) = \frac{\partial}{\partial x} \left( D \frac{\partial u}{\partial x} \right) + g(t, x, u)$$

$0 \leq x \leq 1$ ,  $t > 0$ , that often arise in population dispersal models [12], [19], [22], [23] as well as in more classical applications involving material transport. In the case of species dispersal models, the term involving  $V$  represents a directed movement mechanism (convective, advective, attractive, chemotactic, etc. phenomena),  $D$  is the coefficient of diffusion under the usual Fick's first law formulation, and  $g$  represents general sink/source mechanisms (death/birth, emigration/immigration, etc.) while  $u$  is the population density. Recently such equations (with spatially dependent  $V$  and constant  $D$ ) have been successfully employed in studies of flea beetle movement [12] and transport of labeled substances in brain tissue [12], [28]. However, as pointed out in [12], some of those investigations were limited somewhat by an assumption that  $V$  and  $D$  be constant in time. In the case of insect dispersal, the fact that insects are ectotherms and are very sensitive to weather leads to a natural expectation that their movement rates will vary temporally when observations are taken over several days or more. To model behavior in extended field situations, one must therefore employ equations with time varying coefficients (Example 5.4 in Table 3 of [12] illustrates how dramatically one might expect the estimated diffusion coefficient to vary when determined from experimental data for 1 day vs. that obtained with data for 3 days.) As explained in [12], [23] there are also



situations in which one should allow for spatial dependence in the coefficients.

We present below techniques for estimating nonconstant (i.e., functional) coefficients in a general class of parabolic equations which includes equations such as (1.1) where  $V = V(t, x)$ ,  $D = D(t, x)$ , and  $g(t, x, u) = k(t, x)u$ . We are the first, to our knowledge (e.g., see the surveys [15], [24]), to give a complete treatment consisting of algorithms with convergence proofs as well as numerical results for these variable coefficient estimation problems (some preliminary findings in this area were announced in our earlier note [8]). The methods we develop are based on cubic spline function approximations and can be correctly viewed as extensions of those developed in [7], [12]. However, the fact that we wish to treat non-autonomous systems means that the semigroup approach used in [7], [12] to obtain theoretical convergence results for problems involving autonomous parabolic equations is not directly applicable. (An analogue of the Trotter-Kato convergence theorem -- see [7] -- which can be used to treat evolution equations can be found in the factor space methods developed in [20, Chap. V]; however, the use of an approximating evolution operator framework for the problems under consideration here would not offer any simplification in conceptual or technical details.) Fortunately, an alternate approach that we have employed with success [1], [9], [16], [17] in treating estimation and control problems for delay systems may be applied here, avoiding the semigroup evolution operator theories altogether. Our conceptual framework (in which the "consistency plus stability implies convergence" steps of the Lax Equivalence, Trotter-Kato, factor space theories can also be clearly identified) relies on properties enjoyed by certain approximation schemes when applied to dissipative operators, a simple application of Gronwall's inequality, and basic spline approximation estimates. While we consider only linear systems

in this presentation, our ideas and methods can be extended to also treat estimation and control problems involving certain nonlinear systems of practical interest (for example, see [1], [7], [8], [9], [13], [17]).

In the presentation below we consider systems of the form

$$\frac{\partial u}{\partial t} = q_1(t,x) \frac{\partial^2 u}{\partial x^2} + q_2(t,x) \frac{\partial u}{\partial x} + q_3(t,x)u + f(t,x,q)$$

of which the linear system (1.1) (with  $g = ku$ ) can be shown to be a special case (i.e., carrying out the differentiations in (1.1), we have  $q_1 = \mathcal{D}$ ,  $q_2 = \mathcal{D}_x - \nu$ , and  $q_3 = -\nu_x + k$  so that knowledge of  $q_1, q_2, q_3$  yields  $\mathcal{D}, \nu, k$ ). We first show in section 2 that such systems can be equivalently viewed in an abstract framework; approximate estimation problems are formulated and convergence results given in section 3. In the final section we discuss implementation of the proposed methods and present a summary of our numerical findings for a number of test examples.

## §2. Formulation of the parameter estimation problems

We turn then to consideration of the problem of estimating the vector of unknown variable coefficients,  $q(t,x) = (q_1(t,x), \dots, q_n(t,x))$ , appearing in the parabolic equation

$$(2.1) \quad \frac{\partial u}{\partial t} = q_1(t,x) \frac{\partial^2 u}{\partial x^2} + q_2(t,x) \frac{\partial u}{\partial x} + q_3(t,x)u + f(t,x,q(t,x)),$$

on  $U \equiv (0,T) \times (0,1)$ , with Dirichlet boundary conditions

$$(2.2) \quad u(t,0) = u(t,1) = 0$$

and initial condition

$$(2.3) \quad u(0,x) = \phi(x).$$

We assume throughout that the parameter  $q = (q_1, \dots, q_n)$  belongs to  $Q$ , where  $Q$  is a given compact (in the  $L_2$  topology) subset of

$$\begin{aligned} Q(m,M) \equiv & \left\{ (q_1, \dots, q_n) \in L_2(U) \times \dots \times L_2(U) \mid 0 < m \leq q_1(t,x) \leq M, \right. \\ & \left| \frac{\partial q_1}{\partial x}(t,x) \right| \leq M, |q_j(t,x)| \leq M, \quad j=2,3; \text{ for } i=1,2,\dots,n, \\ & \frac{\partial q_i}{\partial t} \text{ and } \frac{\partial^2 q_i}{\partial x^2} \text{ are uniformly Hölder continuous on } U \text{ with} \\ & \left. \text{exponents in } (0,1) \right\}, \end{aligned}$$

for some positive constants  $m, M$ . We further assume that we are given observations  $\hat{y}_i \in L_2(0,1)$  for the system (2.1)-(2.3) at discrete times  $t_i$ ,  $i = 1, \dots, r$  ( $t_i > 0$ ,  $t_r \leq T$ ), and an output map  $Y(t,x,q) : R \rightarrow R$  such that  $Y$  is continuous in  $q$  and such that the map  $x \rightarrow Y(t_i, x, q)v(x)$  is in  $L_2(0,1)$  whenever  $v \in L_2(0,1)$ . The fundamental identification problem we consider in this paper then consists

of determining a  $\bar{q} \in Q$  that minimizes a distributed least squares fit-to-data functional given by

$$(2.4) \quad J(q) = \sum_{i=1}^r \int_0^1 |\hat{y}_i(x) - Y(t_i, x, q(t_i, x))u(t_i, x; q)|^2 dx,$$

where  $u$  is the solution to (2.1)-(2.3) corresponding to  $q \in Q$ .

We make the following standing assumptions regarding  $Q$  and the system (2.1)-(2.3):

(H1) For each  $q \in Q$  the perturbation function  $g(t, x) = f(t, x, q(t, x))$  is such that  $\frac{\partial g}{\partial t}$  and  $\frac{\partial^2 g}{\partial x^2}$  are uniformly Hölder continuous on  $U$  with exponents in  $(0, 1)$ .

(H2) For each  $q \in Q$ ,  $f(0, 0, q(0, 0)) = f(0, 1, q(0, 1)) = 0$ .

(H3) The function  $q \mapsto f(\cdot, \cdot, q)$  is continuous as a mapping from  $L_2(U) \times \dots \times L_2(U)$  to  $L_2(U)$ .

(H4) The initial function  $\phi$  is in  $H_0^3(0, 1)$ .

Standard results from the theory of parabolic partial differential equations may be called upon to guarantee that, under hypotheses (H1)-(H4), there exists a unique (classical) solution  $u$  (on  $[0, T] \times [0, 1]$ ) to (2.1) to the initial-boundary value problem (2.1)-(2.3) (see, for example, Theorem 7, p. 65 of [18]). In fact, using such results, we find that  $\frac{\partial^2 u}{\partial x^2}$  and  $\frac{\partial u}{\partial t}$  are uniformly continuous functions on  $U$ .

We note that our use of homogeneous boundary conditions (2.2) with equation (2.1) does not restrict the generality of our results since the

corresponding nonhomogeneous boundary value problem,

$$(2.5) \quad \begin{cases} \frac{\partial u}{\partial t} = q_1(t,x) \frac{\partial^2 u}{\partial x^2} + q_2(t,x) \frac{\partial u}{\partial x} + q_3(t,x)u + f(t,x,q(t,x)) \\ u(t,0) = u_0(t) \\ u(t,1) = u_1(t) \\ u(0,x) = \phi(x), \end{cases}$$

can be transformed into

$$(2.6) \quad \begin{cases} \frac{\partial v}{\partial t} = q_1(t,x) \frac{\partial^2 v}{\partial x^2} + q_2(t,x) \frac{\partial v}{\partial x} + q_3(t,x)v + F(t,x,q(t,x)) \\ v(t,0) = v(t,1) = 0 \\ v(0,x) = \phi(x) \end{cases}$$

by letting  $v(t,x) = u(t,x) - (1-x)u_0(t) - xu_1(t)$ . In the event that  $f$  satisfies (H1)-(H3) and, for  $i = 0,1$ ,  $\ddot{u}_i$  is a uniformly Hölder continuous function on  $(0,T)$  satisfying  $u_i(0) = \dot{u}_i(0) = 0$ , it is easy to see that the new perturbing function given by

$$\begin{aligned} F(t,x,q(t,x)) &= f(t,x,q(t,x)) - q_2(t,x)(u_0(t) - u_1(t)) \\ &\quad + q_3(t,x)((1-x)u_0(t) + xu_1(t)) - (1-x)\ddot{u}_0(t) - x\ddot{u}_1(t) \end{aligned}$$

also satisfies hypotheses (H1)-(H3). A similar statement may be made about the case when  $u(t,0) = q_4 u_0(t)$  and  $u(t,1) = q_5 u_1(t)$ , where  $q_4$  and  $q_5$  are (constant) components of the unknown parameter vector  $q$ .

If  $f$  does not depend on  $q$  it is possible to relax the differentiability requirements for  $f$  in the spatial variables (as defined in (H1)) although

modest changes must be made in the theoretical arguments of section 3. For details on the alternative hypotheses and an indication of the required modifications, see Remark 3.1 in that section.

Having stated the fundamental estimation problem, we next consider an abstract setting that might facilitate our treatment of the problem. We shall approximate solutions  $\bar{q}$  of this problem by a sequence  $\{\bar{q}^N\}$  of solutions to estimation problems that are computationally more tractable than our original problem. The approach taken here is similar in spirit to that of a number of other related efforts (see [1], [4], [5], [6], [7], [9], [13] and [16]) in that the original estimation problem is reformulated in a Hilbert space setting where Ritz-Galerkin type ideas may be applied to construct the approximate problems. To this end, we rewrite (2.1)-(2.3) as an abstract evolution equation (AEE) in an infinite-dimensional state space; although the use of spaces and operators here is quite standard and well-established in the literature, the dependence of our problem on unknown parameters requires that we make an effort to carefully define the operators involved.

Define  $Z = L_2(0,1)$  with the usual inner product  $\langle \cdot, \cdot \rangle$  and norm  $|\cdot|$ . For  $q = (q_1, \dots, q_n) \in Q$ , and  $t \in [0, T]$ , let the operator  $A(t, q) : \mathcal{D} \rightarrow Z$  be given by

$$(2.7) \quad A(t, q)\psi = q_1(t, \cdot)D^2\psi + q_2(t, \cdot)D\psi + q_3(t, \cdot)\psi$$

for  $\psi \in \text{dom}(A(t, q)) = \mathcal{D} \equiv H^2(0,1) \cap H_0^1(0,1)$ , where  $D = \frac{\partial}{\partial x}$  is the usual differentiation operator. Finally, for each  $q \in Q$  and  $t \in [0, T]$ , define

$G(t, q) = f(t, \cdot, q(t, \cdot)) \in Z$ . Before we give the equivalence between (2.1)-(2.3) and an AEE on  $Z$ , we shall establish, for the operator  $A(t, q)$ , a dissipative inequality that is fundamental to the calculations that follow.

Lemma 2.1. There is a constant  $\omega > 0$  such that

$$(2.8) \quad \langle A(t, q)\psi, \psi \rangle \leq \omega |\psi|^2$$

for all  $\psi \in \mathcal{D}$ , uniformly in  $t \in [0, T]$  and  $q \in Q$ .

Proof: For  $\psi \in \mathcal{D}$ ,  $q \in Q$  and  $t \in [0, T]$ ,

$$\langle A(t, q)\psi, \psi \rangle = \langle q_1 D^2 \psi, \psi \rangle + \langle q_2 D\psi, \psi \rangle + \langle q_3 \psi, \psi \rangle,$$

where  $q_i$  is understood to mean  $q_i(t, \cdot)$  for  $i = 1, 2, 3$ . Using integration by parts and the boundary conditions on  $\psi$  we obtain

$$\begin{aligned} \langle q_1 D^2 \psi, \psi \rangle &= - \langle D\psi, D(q_1 \psi) \rangle \\ &= - \langle D\psi, q_1 D\psi \rangle - \langle D\psi, (Dq_1) \psi \rangle \\ &= - |q_1^{1/2} D\psi|^2 - \langle q_1^{1/2} D\psi, \frac{1}{q_1^{1/2}} (Dq_1) \psi \rangle \\ &\leq - |q_1^{1/2} D\psi|^2 + |q_1^{1/2} D\psi| \left| \frac{1}{q_1^{1/2}} (Dq_1) \psi \right| \\ &\leq - |q_1^{1/2} D\psi|^2 + \frac{1}{2} |q_1^{1/2} D\psi|^2 + \frac{1}{2} \left| \frac{1}{q_1^{1/2}} (Dq_1) \psi \right|^2 \\ &\leq - \frac{1}{2} |q_1^{1/2} D\psi|^2 + \frac{1}{2} \left| \frac{1}{q_1^{1/2}} (Dq_1) \psi \right|^2. \end{aligned}$$

In addition,

$$\begin{aligned} \langle q_2 D\psi, \psi \rangle &= \langle q_1^{1/2} D\psi, \frac{q_2}{q_1^{1/2}} \psi \rangle \\ &\leq \frac{1}{2} |q_1^{1/2} D\psi|^2 + \frac{1}{2} \left| \frac{q_2}{q_1^{1/2}} \psi \right|^2. \end{aligned}$$

Combining these estimates with bounds on  $q_i$ ,  $i = 1, 2, 3$ , and  $\frac{\partial q_1}{\partial x}$  given in the definition of  $Q$ , we find

$$\begin{aligned} \langle A(t, q)\psi, \psi \rangle &\leq \frac{1}{2} \left| \frac{1}{q_1^{1/2}} \right| (Dq_1) |\psi|^2 + \frac{1}{2} \left| \frac{q_2}{q_1^{1/2}} \right| |\psi|^2 + M |\psi|^2 \\ &\leq \left( \frac{M^2}{m} + M \right) |\psi|^2 \end{aligned}$$

so that  $\omega = \frac{M^2}{m} + M$  can be chosen independent of  $t$  and  $q \in Q$ .

In the theorem that follows we establish the equivalence between (2.1)-(2.3) and an AEE on  $Z$ , obtaining some needed continuous dependence results as well.

Theorem 2.1 Let  $q \in Q$  be fixed and let  $y(t, q) = u(t, \cdot; q)$  where  $(t, x) \rightarrow u(t, x; q)$  is the solution to (2.1)-(2.3) on  $U$ . Then  $y$  is also the unique solution on  $[0, T]$  of

$$(2.9) \quad z(t) = \phi + \int_0^t \{A(\sigma, q)z(\sigma) + G(\sigma, q)\} d\sigma.$$

Furthermore  $y(t; q) \in Z$  is continuous in  $t \in [0, T]$  and uniformly continuous in  $\phi \in H_0^3$  (in the  $Z$  topology), uniformly in  $t \in [0, T]$  and  $q \in Q$ .

Proof: That  $t \rightarrow y(t; q)$  satisfies (2.9) follows immediately from the definitions of the operators involved and the comments following (H1)-(H4). The arguments required to establish uniqueness are similar to those for continuous dependence, so we present only the estimates that prove the latter.

If  $z$  and  $\tilde{z}$  denote solutions to (2.9) associated with  $\phi$  and  $\tilde{\phi}$  (in  $H_0^3$ ) respectively, then



$$(2.10) \quad z(t) - \tilde{z}(t) = \phi - \tilde{\phi} + \int_0^t \{A(\sigma, q)z(\sigma) - A(\sigma, q)\tilde{z}(\sigma)\} d\sigma.$$

We require an integral version of the well-known result [14, p. 100] that  $\frac{d}{dt} \frac{1}{2} |x(t)|^2 = \langle \dot{x}(t), x(t) \rangle$ . If  $X$  is a Hilbert space and if  $x: [a, b] \rightarrow X$  is given by  $x(t) = x(a) + \int_a^t v(\sigma) d\sigma$ , then

$$(2.11) \quad |x(t)|^2 = |x(a)|^2 + 2 \int_a^t \langle v(\sigma), x(\sigma) \rangle d\sigma.$$

In our case we find, using (2.10) and this result, that

$$\begin{aligned} |z(t) - \tilde{z}(t)|^2 &= |\phi - \tilde{\phi}|^2 + 2 \int_0^t \langle A(\sigma, q)(z(\sigma) - \tilde{z}(\sigma)), z(\sigma) - \tilde{z}(\sigma) \rangle d\sigma \\ &\leq |\phi - \tilde{\phi}|^2 + 2\omega \int_0^T |z(\sigma) - \tilde{z}(\sigma)|^2 d\sigma, \end{aligned}$$

where we have used the dissipative property for  $A(\sigma, q)$  that is uniform in  $\sigma$  and  $q$ . Finally, an application of Gronwall's inequality yields

$$|z(t) - \tilde{z}(t)|^2 \leq |\phi - \tilde{\phi}|^2 \exp(2\omega T),$$

and the desired continuity result (uniform in  $t$  and  $q$ ) obtains.

In view of the established equivalence, the parameter estimation problem involving (2.4) may be reformulated as an abstract identification problem, where we now wish to find  $\bar{q} \in Q$  that minimizes

$$(2.12) \quad J(q) = \sum_{i=1}^r \left| \hat{y}_i - c(t_i, q)z(t_i; q) \right|^2$$

where  $z$  is the solution to (2.9) corresponding to  $q \in Q$ ,  $C(t, q) : Z \rightarrow Z$  is defined by  $C(t, q)\psi = Y(t, \cdot, q(t, \cdot))\psi$ , for  $\psi \in Z$ , and  $|\cdot|$  is the usual  $L_2(0, 1)$  norm.

**Theorem 2.2.** There is a solution  $\bar{q}$  in  $Q$  to the parameter estimation problem for (2.9), (2.12) (equivalently, (2.1)-(2.3), (2.4)).

**Proof:** In the arguments that follow, we shall show that the map  $q \rightarrow z(t; q)$  is continuous for each  $t \in (0, T)$ , so that the continuity of  $q \rightarrow J(q)$  is assured; therefore, there is a parameter  $\bar{q}$  in the compact set  $Q$  for which  $J$  attains its minimum.

Let  $q, \hat{q}$  be given in  $Q$  and let  $z, \hat{z}$  be the corresponding solutions to (2.9). Applying (2.11) we find that

$$\begin{aligned}
 |z(t) - \hat{z}(t)|^2 &= 2 \int_0^t \langle A(\sigma, q) - A(\sigma, \hat{q}) \rangle z(\sigma), z(\sigma) - \hat{z}(\sigma) \rangle d\sigma \\
 &\quad + 2 \int_0^t \langle A(\sigma, \hat{q}) \rangle (z(\sigma) - \hat{z}(\sigma)), z(\sigma) - \hat{z}(\sigma) \rangle d\sigma \\
 &\quad + 2 \int_0^t \langle G(\sigma, q) - G(\sigma, \hat{q}) \rangle, z(\sigma) - \hat{z}(\sigma) \rangle d\sigma \\
 &\leq 2 \int_0^t |(A(\sigma, q) - A(\sigma, \hat{q}))z(\sigma)| |z(\sigma) - \hat{z}(\sigma)| d\sigma \\
 &\quad + 2\omega \int_0^t |z(\sigma) - \hat{z}(\sigma)|^2 d\sigma \\
 &\quad + 2 \int_0^t |G(\sigma, q) - G(\sigma, \hat{q})| |z(\sigma) - \hat{z}(\sigma)| d\sigma \\
 &\leq \int_0^T |(A(\sigma, q) - A(\sigma, \hat{q}))z(\sigma)|^2 d\sigma \\
 &\quad + \int_0^T |G(\sigma, q) - G(\sigma, \hat{q})|^2 d\sigma \\
 &\quad + 2(\omega+1) \int_0^T |z(\sigma) - \hat{z}(\sigma)|^2 d\sigma,
 \end{aligned}$$

where dissipativeness for  $A(\sigma, q)$  has been used, along with the inequality  $2ab \leq a^2 + b^2$  that holds for  $a$  and  $b$  real numbers. Applying Gronwall's inequality to the last expression we see that the continuity result depends on estimates for the first term (that the second term involving  $G$  may be made arbitrarily small is immediate from (H3)). To this end, we observe that

$$\begin{aligned}
 (2.13) \quad \int_0^T |(A(\sigma, q) - A(\sigma, \tilde{q}))z(\sigma)|^2 d\sigma &\leq 2 \int_0^T |(q_1(\sigma, \cdot) - \tilde{q}_1(\sigma, \cdot))D^2 z(\sigma)|^2 d\sigma \\
 &\quad + 4 \int_0^T |(q_2(\sigma, \cdot) - \tilde{q}_2(\sigma, \cdot))Dz(\sigma)|^2 d\sigma \\
 &\quad + 4 \int_0^T |(q_3(\sigma, \cdot) - \tilde{q}_3(\sigma, \cdot))z(\sigma)|^2 d\sigma \\
 &\leq 4(N_2^2 + N_1^2 + N_0^2) |q - \tilde{q}|^2
 \end{aligned}$$

where in the last expression  $|\cdot|$  denotes the  $L_2(U) \times \dots \times L_2(U)$  norm and  $N_i = \sup\{|(D^i z(\sigma))(x)| : \sigma \in (0, T), x \in (0, 1)\}$  is finite,  $i = 0, 1, 2$ , (see the comments following (H1)-(H4) above). The continuity of  $J$  and thus the existence results are established.

We remark that the important aspect of the above result is the continuous dependence of  $z$  on  $q$  which is needed to establish existence of solutions to the approximate estimation problems formulated in the next section (see Theorem 3.2). Indeed, existence of solutions to our original estimation problem follows from the convergence results for sequences of solutions to the approximate problems (see Theorem 3.5).

### §3 Approximate parameter estimation problems

We focus in this section on the problem of approximating the infinite-dimensional estimation problem for (2.9), (2.12) by a sequence of parameter estimation problems for which the state variable satisfies an ordinary differential equation (ODE) on a finite-dimensional state space  $Z^N$ . Fundamental to this undertaking is the task of establishing the convergence of solutions of the approximating systems on  $Z^N$  to solutions of the original AEE on  $Z$ . Although our formulation is a classical one of the Ritz type (involving orthogonal projections of an infinite-dimensional system onto a sequence of finite-dimensional subspaces) that is modified to allow for  $q$ -dependent operators and variables, our calculations are much simpler than those for functional differential equations in [4], [9] and [16], where the spaces  $Z$  and  $Z^N$  as well depend on the choice of  $q$ .

For the approximation spaces  $Z^N$ , we take the spans of cubic spline basis elements which have been modified so as to satisfy the homogeneous boundary conditions. Specifically, for any integer  $N > 0$ , let  $x_j^N = j/N$ ,  $j = -3, \dots, N+3$ , and  $S_j^N$ ,  $j = -1, \dots, N+1$ , be the cubic spline that vanishes outside  $(x_{j-2}^N, x_{j+2}^N)$ , has value 4 and slope 0 at  $x_j^N$ , value 1 and slope  $3N$  at  $x_{j-1}^N$ , and value 1 and slope  $-3N$  at  $x_{j+1}^N$ . Then  $S_j^N$  is the standard cubic spline found in the literature (see, for example, [27, p. 73] where the basis elements differ from the ones defined here by a factor of 24). We note that for some values of  $j$  we do not have  $S_j^N$  satisfying homogeneous boundary conditions. The modified basis elements  $B_j^N$  considered here will be the restriction to  $[0,1]$  of the following functions:

$$B_0^N = S_0^N - 4S_{-1}^N$$

$$B_1^N = S_0^N - 4S_1^N$$

$$B_j^N = S_j^N, \quad j = 2, \dots, N-2$$

$$B_{N-1}^N = S_N^N - 4S_{N-1}^N$$

$$B_N^N = S_N^N - 4S_{N+1}^N.$$

The approximating subspaces  $Z^N$  of  $Z$  are then given by  $Z^N = \text{span}\{B_0^N, \dots, B_N^N\}$ , for which it is easy to see that  $Z^N \subset \mathcal{D}$  for each  $N = 1, 2, \dots$ .

Our intermediate goal is to find approximations, for fixed  $q \in Q$ , to the solution  $z$  on  $[t_1, T]$  of

$$(3.1) \quad z(t; q) = z(t_1; q) + \int_{t_1}^t \{A(\sigma, q)z(\sigma; q) + G(\sigma, q)\} d\sigma,$$

which is equivalent to (2.9) if  $z(t_1; q)$  is given by (2.9) for time  $t_1 > 0$  (the first sampling time). To this end we define, for  $t \in [t_1, T]$

$$(3.2) \quad z^N(t; q) = P^N z(t_1; q) + \int_{t_1}^t \{A^N(\sigma, q)z^N(\sigma; q) + P^N G(\sigma, q)\} d\sigma,$$

where  $P^N: Z \rightarrow Z^N$  is the orthogonal projection characterized by  $\langle P^N z - z, B_j^N \rangle = 0$ ,  $j = 0, 1, \dots, N$ , and  $A^N: Z \rightarrow Z^N$  is defined by  $A^N(t, q) = P^N A(t, q) P^N$ . Since  $z^N(t)$  in (3.2) belongs to  $Z^N$ , a finite-dimensional space, equation (3.2) is equivalent to the ODE on  $[t_1, T]$

$$(3.3) \quad \begin{cases} \dot{z}^N(t; q) = A^N(t, q)z^N(t; q) + P^N G(t, q), \\ z^N(t_1; q) = P^N z(t_1; q) \end{cases}$$

which, as we shall show in the arguments to follow, approximates (3.1) in some sense. We remark here that although  $\phi$  does not explicitly appear in (3.2) and (3.3),  $z^N$  depends on  $\phi$  in that  $z^N(t_1)$  was generated using  $z(t_1)$  from (2.9) with  $z(0) = \phi$ .

Associated with (3.2) (or (3.3)) is an "approximate parameter estimation problem": Find  $\bar{q}^N \in Q$  that minimizes

$$(3.4) \quad J^N(q) = \sum_{i=1}^r |\hat{y}_i - c(t_i; q) z^N(t_i; q)|^2$$

where  $z^N$  is the solution to (3.3) corresponding to  $q \in Q$ .

Before discussing the convergence of  $z^N(t)$  to  $z(t)$  as  $N \rightarrow \infty$ , we establish analogues of Lemma 2.1 and Theorem 2.1 for the operator  $A^N$  and the  $N^{\text{th}}$  ODE (3.3), respectively. Our first result is a dissipative property for  $A^N$  that follows immediately from the same property for  $A$ ; that is, for any  $\psi^N \in Z^N$ ,

$$\begin{aligned} \langle A^N(t, q) \psi^N, \psi^N \rangle &= \langle P^N A(t, q) P^N \psi^N, \psi^N \rangle \\ &= \langle A(t, q) P^N \psi^N, P^N \psi^N \rangle \\ &\leq \omega |\psi^N|^2 \end{aligned}$$

where we have used the fact that  $P^N$  is self-adjoint. We summarize this finding in the following.

Lemma 3.1. Let  $\omega = \frac{M^2}{m} + M > 0$ . Then, for every  $\psi^N \in Z^N$ ,

$$(3.5) \quad \langle A^N(t, q) \psi^N, \psi^N \rangle \leq \omega |\psi^N|^2$$

for all  $t \in [0, T]$  and  $q \in Q$ , and for each  $N = 1, 2, \dots$ .

Our next result guarantees the existence of solutions to (3.3) as well as to the  $N^{\text{th}}$  parameter estimation problem. Furthermore, in the proof of the former we outline the numerical scheme used to solve (3.3) for various sample problems reported in section 4.

Theorem 3.1. Let  $q$  be fixed in  $Q$ . Then there exists a unique solution  $z^N$  to (3.3) on  $[t_1, T]$  that depends continuously on  $\phi \in H_0^3$  (in the  $L_2(0,1)$  topology), uniformly in  $t \in [t_1, T]$ ,  $q \in Q$ , and  $N = 1, 2, \dots$ .

Proof: Our arguments are similar to those developed in [9], [11], where  $z^N(t)$  is written in terms of the basis elements  $\{B_j^N\}$  for  $Z^N$ .

Define  $\beta^N$  as the  $1 \times (N+1)$  row vector function given by

$$\beta^N = (B_0^N, \dots, B_N^N).$$

For each  $t \in [t_1, T]$ ,  $z^N(t) \in Z^N$ , so that there exists  $w^N(t) \in R^{N+1}$ ,  $w^N(t) = \text{col}(w_0^N(t), \dots, w_N^N(t))$  such that  $z^N(t) = \beta^N w^N(t)$ . Thus we may rewrite (3.3) as

$$(3.6) \quad \begin{cases} \dot{\beta}^N w^N(t) = A^N(t, q) \beta^N w^N(t) + \beta^N g^N(t), & t \in [t_1, T], \\ \beta^N w^N(t_1) = \beta^N \zeta^N \end{cases}$$

where  $\zeta^N$  and  $g^N(t)$  in  $R^{N+1}$  are defined by  $P^N z(t_1) = \beta^N \zeta^N$  and  $P^N G(t) = \beta^N g^N(t)$ ; it is understood that  $w^N$ ,  $g^N$ , and  $\zeta^N$  depend on  $q \in Q$ . Let  $A^N(t, q)$  denote the matrix representation of  $A^N(t, q)$  with respect to the basis elements  $\{B_0^N, \dots, B_N^N\}$ . Then usual Galerkin arguments establish that the coefficients  $w^N(t)$  in (3.6) satisfy

$$(3.7) \quad \begin{cases} \dot{w}^N(t) = A^N(t, q) w^N(t) + g^N(t), & t \in [t_1, T], \\ w^N(t_1) = \zeta^N, \end{cases}$$

so that once we determine  $A^N(t,q)$  we will be able to analyze the existence and uniqueness of solutions to (3.7); in addition, the realization of numerical algorithms to solve our approximate estimation problem will be based on (3.7). Note that for any  $\psi \in Z$ ,  $(P^N_\psi - \psi) \in (Z^N)^\perp$  so that for each  $j = 0, \dots, N$ ,

$$\langle P^N_\psi - \psi, B_j^N \rangle = 0,$$

or, equivalently,

$$(3.8) \quad \langle \psi, B_j^N \rangle = \langle P^N_\psi, B_j^N \rangle.$$

However, since there exists  $\xi^N = (\xi_0^N, \dots, \xi_N^N)^T \in R^{N+1}$  such that

$$(3.9) \quad P^N_\psi = \beta_{\xi^N}^N,$$

equation (3.8) can be written

$$\begin{aligned} \langle \psi, B_j^N \rangle &= \langle \beta_{\xi^N}^N, B_j^N \rangle \\ &= \sum_{i=0}^N \langle B_i^N, B_j^N \rangle \xi_i^N, \quad j = 0, \dots, N. \end{aligned}$$

This may be written as a matrix equation

$$H^N(\psi) = Q_{\xi^N}^N$$

where

$$H^N(\psi) = \begin{pmatrix} \langle \psi, B_0^N \rangle \\ \vdots \\ \langle \psi, B_N^N \rangle \end{pmatrix}$$

and the  $(N+1)$  square matrix  $Q^N$  has elements  $Q_{i,j}^N = \langle B_i^N, B_j^N \rangle$ ,  $i, j = 0, 1, \dots, N$ .



It follows that we may solve for  $\xi^N$  by writing

$$(3.10) \quad \xi^N = (Q^N)^{-1} H^N(\psi),$$

where  $Q^N$  is invertible since it is the Gramian of linearly independent basis elements for  $Z^N$ . The desired representation for  $A^N(t, q)$  may be derived from these estimates since

$$\begin{aligned} A^N(t, q) z^N(t) &= P^N A(t, q) \beta^N w^N(t) \\ &= P^N [q_1(t, \cdot) D^2(\beta^N w^N(t)) + q_2(t, \cdot) D(\beta^N w^N(t)) + q_3(t, \cdot) \beta^N w^N(t)] \\ &= \beta^N \alpha^N(t) \end{aligned}$$

for some  $\alpha^N(t) \in R^{N+1}$ . Thus, applying (3.9) and (3.10), we find

$$\begin{aligned} \alpha^N(t) &= (Q^N)^{-1} H^N \left( q_1(t, \cdot) D^2(\beta^N w^N(t)) + q_2(t, \cdot) D(\beta^N w^N(t)) + q_3(t, \cdot) \beta^N w^N(t) \right) \\ &= (Q^N)^{-1} \begin{pmatrix} \sum_{j=0}^N w_j^N(t) \langle q_1(t, \cdot) D^2 \beta_j^N, \beta_0^N \rangle \\ \vdots \\ \sum_{j=0}^N w_j^N(t) \langle q_1(t, \cdot) D^2 \beta_j^N, \beta_N^N \rangle \end{pmatrix} \\ &\quad + (Q^N)^{-1} \begin{pmatrix} \sum_{j=0}^N w_j^N(t) \langle q_2(t, \cdot) D \beta_j^N, \beta_0^N \rangle \\ \vdots \\ \sum_{j=0}^N w_j^N(t) \langle q_2(t, \cdot) D \beta_j^N, \beta_N^N \rangle \end{pmatrix} \end{aligned}$$

$$\begin{aligned}
& + (Q_N)^{-1} \begin{pmatrix} \sum_{j=0}^N w_j^N(t) \langle q_3(t, \cdot) B_j^N, B_0^N \rangle \\ \vdots \\ \sum_{j=0}^N w_j^N(t) \langle q_3(t, \cdot) B_j^N, B_N^N \rangle \end{pmatrix} \\
& = (Q_N)^{-1} (K_1^N(q) + K_2^N(q) + K_3^N(q)) w^N(t) .
\end{aligned}$$

Here the  $(N+1)$ -square matrices  $K_1^N$ ,  $K_2^N$ , and  $K_3^N$  have elements given by

$$K_1^N(q)_{i,j} = \langle q_1(t, \cdot) D^2 B_j^N, B_i^N \rangle ,$$

$$K_2^N(q)_{i,j} = \langle q_2(t, \cdot) D B_j^N, B_i^N \rangle ,$$

$$K_3^N(q)_{i,j} = \langle q_3(t, \cdot) B_j^N, B_i^N \rangle .$$

Hence we may conclude that (3.7) may be rewritten as a linear  $(N+1)$ -vector ODE in  $w^N(t)$  for  $t \in [t_1, T]$ ,

$$(3.11) \quad \begin{cases} \dot{w}^N(t) = (Q^N)^{-1} (K_1^N(q) + K_2^N(q) + K_3^N(q)) w^N(t) + g^N(t), \\ w^N(t_1) = \zeta^N . \end{cases}$$

We may then apply standard differential equation theory to obtain the existence of a unique solution of (3.11) on  $[t_1, T]$  that depends continuously on  $\zeta^N$ .

Moreover, since

$$\zeta^N = (Q^N)^{-1} H^N(z(t_1)) ,$$

where the well-defined map  $\phi \rightarrow z(t_1)$  is continuous, it follows that the solution to (3.3) given by

$$z^N(t) = \beta_{w^N}^N(t),$$

is unique on  $[t_1, T]$  and continuously dependent on  $\phi \in H_0^3$ . We have only to show that the continuity is uniform in  $t \in [t_1, T]$ ,  $q \in Q$ , and  $N = 1, 2, \dots$ . This follows easily from the (uniform) dissipative result for  $A^N$ , as the required arguments are virtually the same as those used to demonstrate the continuity (uniform in  $t, q$ ) of  $\phi \rightarrow z(t; q)$  (found in the proof of Theorem 2.1).

Finally, minor modifications in the proof of Theorem 2.2 yield the following. (Note we use here the continuity of  $q \rightarrow z(t_1; q)$ .)

Theorem 3.2: The  $N^{\text{th}}$  approximate parameter estimation problem has a solution  $\bar{q}^N \in Q$  for each  $N = 1, 2, \dots$ .

We may, therefore, determine a solution  $\bar{q}^N$  to the  $N^{\text{th}}$  identification problem by applying conventional optimization techniques with computational schemes that solve (3.11) (the ODE in the "Fourier" coefficients  $w^N(t)$ ). Although we may be able to determine  $\bar{q}^N$  fairly easily in the  $N^{\text{th}}$  ODE-governed problem (especially for small values of  $N$ ), the solution  $\bar{q}^N$  we find is meaningful only if  $\bar{q}^N$  approximates the desired solution  $\bar{q}$  to the original estimation problem. Fundamental to the establishment of this fact (i.e., the convergence of  $\bar{q}^N$  to  $\bar{q}$  in some sense) is the demonstration that  $z^N(t; q^N) \rightarrow z(t; \check{q})$  for any sequence  $\{q^N\}$  of parameters in  $Q$  that converges to some  $\check{q} \in Q$ .

To pursue this line of argument, we shall therefore assume that an arbitrary sequence  $\{q^N\}$  of parameter functions has been given such that  $q^N \rightarrow \tilde{q}$  in the  $L_2(U) \times \dots \times L_2(U)$  topology, where  $\tilde{q}$  and  $q^N \in Q$ ,  $N = 1, 2, \dots$ . We first consider the problem of obtaining the convergence of  $z^N(t; q^N)$  to  $z(t; \tilde{q})$  for initial data  $\phi$  in a smooth but dense subset of  $H_0^3$ , a restriction that simplifies our calculations since we are able to take advantage of several useful spline estimates (given below).

Let  $\mathcal{Z}$  denote the subspace of  $Z$  given by  $\mathcal{Z} = H^4 \cap H_0^1$ . Then for  $\psi \in \mathcal{Z}$  we obtain the spline estimates presented in Lemma 3.2 below, the proof of which may be found in [7, Lemma 2.3] (the arguments use standard techniques from spline analysis such as those underlying Theorem 6.13 of [27]).

Lemma 3.2 Let  $\psi$  be given in  $Z$ . Then

$$(3.12) \quad |P^N \psi - \psi| \leq \frac{C_0}{N^4} |D^4 \psi|,$$

$$(3.13) \quad |D(P^N \psi - \psi)| \leq \frac{C_1}{N^3} |D^4 \psi|, \text{ and}$$

$$(3.14) \quad |D^2(P^N \psi - \psi)| \leq \frac{C_2}{N^2} |D^4 \psi|,$$

where  $C_0, C_1, C_2$  are constants independent of  $\psi$  and  $N$ .

We turn now to a rather technical result that facilitates later convergence proofs. To argue that  $z^N(t; q^N) \rightarrow z(t; \tilde{q})$ , we shall need to use estimates such as (3.12)-(3.14) where  $\psi = z(t; \tilde{q})$  and hence need conditions under which  $z(t; \tilde{q}) \in \mathcal{Z}$ . This can be guaranteed if we suitably restrict the initial data for  $z$ . To this end we define  $I = H^6 \cap H_0^3$  and note that  $I$  is dense in the initial data set  $H_0^3$  (in the  $L_2$  topology). We can then prove the following.

**Lemma 3.3** Suppose  $q \in Q$  is fixed and let  $\phi$  be given in  $I$ . Then the solution  $z$  to (3.1) corresponding to the initial data  $\phi$  is such that  $z(t;q) \in \mathcal{Z}$  for each  $t \in [t_1, t_r]$ .

**Proof:** We shall need certain results from Chapter 3 of [18]. From (H1) and the definition of  $Q$  it follows that for  $i = 1, \dots, n$ , and  $s = 0, 1, 2$ ,  $\frac{\partial q_i}{\partial x^s}$ ,  $\frac{\partial^s q_i}{\partial x^s}$ ,  $\frac{\partial q}{\partial t}$ , and  $\frac{\partial^s g}{\partial x^s}$  (where  $g(t, x) = f(t, x, q(t, x))$ ) are uniformly Hölder continuous functions on  $U$  with exponents in  $(0, 1)$ . Pick  $\alpha \in (0, 1)$  as the maximum of these exponents so that each function is uniformly Hölder continuous with exponent  $\alpha$ .

If  $\phi \in I$  is given,  $\phi$  belongs to  $C^5(0, 1)$  so that, for  $s = 0, \dots, 4$ ,  $D^s \phi$  has a bounded (continuous) derivative on  $(0, 1)$ . It follows immediately that  $D^s \phi$ ,  $s = 0, \dots, 4$ , are uniformly Hölder continuous on  $(0, 1)$  with exponent  $\alpha$ . In addition,  $\phi \in I$  implies that  $\phi \in H_0^3$  so that  $(D^2 \phi)(x) = (D \phi)(x) = \phi(x) = 0$  for  $x = 0, 1$ . Therefore, for  $x = 0, 1$ , and  $t = 0$ ,

$$A(t, q)\phi(x) + G(t, q)(x) = 0 ,$$

where we have used hypothesis (H2) to set the second term equal to zero.

We note that this last condition is just the condition " $L\psi = f$  on  $\partial B$ " in the notation of [18, p. 75].

Standard regularity theorems for parabolic equations may now be applied: Specifically, one may use Corollary 1 of [18, p. 78] (with  $p = 1$  in the notation of [18]) to make minor modifications in the arguments underlying Theorem 12, p. 75, of the same reference (with  $p = 2$  for the spatial derivatives) and conclude that  $D^4 z(t; q)$  is uniformly Hölder continuous on  $(0, 1)$  (with exponent  $\alpha$ ) for every  $t \in [t_1, t_r]$ .

The preceding results may now be employed to demonstrate convergence of  $z^N(t; q^N)$  to  $z(t; \tilde{q})$  whenever  $z(t; \tilde{q}) \in \mathcal{J}$ ; i.e., when  $\phi \in I$  and  $t \in [t_1, t_r]$ .

**Theorem 3.3:** Let  $\phi \in I$  be given. Suppose  $\{q^N\}$  is arbitrary in  $Q$  with  $q^N \rightarrow \tilde{q}$  and  $\tilde{q} \in Q$ . Then

$$z^N(t; q^N) \rightarrow z(t; \tilde{q})$$

as  $N \rightarrow \infty$ , uniformly in  $t \in [t_1, t_r]$ .

**Proof:** Where no confusion results, we shall let  $z^N(t)$  and  $z(t)$  represent the solutions to (3.2) and (3.1) corresponding to  $q^N$  and  $\tilde{q}$ , respectively. Then for  $t \in [t_1, t_r]$ ,

$$(3.15) \quad |z^N(t) - z(t)| \leq |z^N(t) - p^N z(t)| + |p^N z(t) - z(t)|$$

where the second term converges to zero as  $N \rightarrow \infty$  from (3.12) and Lemma 3.3; in fact, convergence is uniform in  $t$  due to the compactness of  $\{z(t) | t \in [t_1, t_r]\}$  in  $Z$ . It remains to consider  $|z^N(t) - p^N z(t)|$ . From (3.1), (3.2) and (2.11) we have

$$\begin{aligned} |z^N(t) - p^N z(t)|^2 &= |p^N z(t_1; q^N) - p^N z(t_1; \tilde{q})|^2 \\ &\quad + 2 \int_{t_1}^t \langle A^N(\sigma, q^N)(z^N(\sigma) - p^N z(\sigma)), z^N(\sigma) - p^N z(\sigma) \rangle d\sigma \\ &\quad + 2 \int_{t_1}^t \langle A^N(\sigma, q^N)p^N z(\sigma) - p^N A(\sigma, \tilde{q})z(\sigma), z^N(\sigma) - p^N z(\sigma) \rangle d\sigma \\ &\quad + 2 \int_{t_1}^t \langle p^N G(\sigma, q^N) - p^N G(\sigma, \tilde{q}), z^N(\sigma) - p^N z(\sigma) \rangle d\sigma. \end{aligned}$$

Appealing to arguments similar to those found in the proof of Theorem 2.2, we thus argue

$$(3.16) \quad |z^N(t) - p^N z(t)|^2 \leq T_1(N) + T_2(N) + T_3(N) + 2(\omega+1) \int_{t_1}^{t_r} |z^N(\sigma) - p^N z(\sigma)|^2 d\sigma ,$$

where

$$T_1(N) \equiv |z(t_1; q^N) - z(t_1; \tilde{q})|^2 ,$$

$$T_2(N) \equiv \int_{t_1}^{t_r} |A^N(\sigma, q^N) p^N z(\sigma) - p^N A(\sigma, \tilde{q}) z(\sigma)|^2 d\sigma ,$$

$$T_3(N) \equiv \int_{t_1}^{t_r} |G(\sigma, q^N) - G(\sigma, \tilde{q})|^2 d\sigma .$$

It remains only to verify that  $T_i(N) \rightarrow 0$  as  $N \rightarrow \infty$ ,  $i = 1, 2, 3$ ; an application of the Gronwall inequality to (3.16) will then give the desired convergence of  $|z^N(t) - p^N z(t)|$  to zero as  $N \rightarrow \infty$ , uniformly in  $t \in [t_1, t_r]$ .

The convergence of  $T_1(N)$  to zero is an immediate consequence of the proof of Theorem 2.2. In addition,  $T_3(N) \rightarrow 0$  from (H3). Further,  $T_2(N) \leq 2\tau_1(N) + 2\tau_2(N)$  where

$$\tau_1(N) \equiv \int_{t_1}^{t_r} |A^N(\sigma, q^N) p^N z(\sigma) - p^N A(\sigma, q^N) z(\sigma)|^2 d\sigma$$

and

$$\tau_2(N) \equiv \int_{t_1}^{t_r} |p^N A(\sigma, q^N) z(\sigma) - p^N A(\sigma, \tilde{q}) z(\sigma)|^2 d\sigma$$

converge to zero as  $N \rightarrow \infty$ , (the argument for  $\tau_2$  follows the reasoning of (2.13)). Considering  $\tau_1$ , we first observe that the integrand satisfies

$$\begin{aligned}
& |(P^N A(\sigma, q^N) P^N) P^N z(\sigma) - P^N A(\sigma, q^N) z(\sigma)| \\
& \leq |A(\sigma, q^N)(P^N z(\sigma) - z(\sigma))| \\
& \leq |q_1^N(\sigma, \cdot) D^2(P^N z(\sigma) - z(\sigma))| + |q_2^N(\sigma, \cdot) D(P^N z(\sigma) - z(\sigma))| \\
& \quad + |q_3^N(\sigma, \cdot)(P^N z(\sigma) - z(\sigma))| \\
& \leq M \left( \frac{C_2}{N^2} + \frac{C_1}{N^3} + \frac{C_0}{N^4} \right) |D^4 z(\sigma; \tilde{q})| \\
& \equiv \Theta^N(\sigma)
\end{aligned}$$

from (3.12), (3.13), (3.14) and the definition of  $Q$ . Furthermore, the convergence of  $\Theta^N(\sigma) \rightarrow 0$  as  $N \rightarrow \infty$  is dominated since

$$\Theta^N(\sigma) \leq M(C_0 + C_1 + C_2) |D^4 z(\sigma; \tilde{q})| ,$$

where the map  $\sigma \rightarrow |D^4 z(\sigma; \tilde{q})|$  is in  $L_2(t_1, t_r)$  since  $\phi \in I$  (the arguments are similar to those used to prove Lemma 3.3; i.e., the map  $(\sigma, x) \rightarrow D^4 z(\sigma; \tilde{q})(x)$  is uniformly Hölder continuous on  $(t_1, t_r) \times (0, 1)$ ).

Finally, we are able to derive state variable convergence for arbitrary  $\phi \in H_0^3$ .

Theorem 3.4: Suppose that  $q^N \rightarrow \tilde{q}$  where  $q^N$  and  $\tilde{q}$  are arbitrary in  $Q$ . Then for any  $\phi \in H_0^3$ ,

$$z^N(t; q^N) \rightarrow z(t; \tilde{q})$$

as  $N \rightarrow \infty$ , uniformly in  $t \in [t_1, t_r]$ .



Proof: Since  $I$  is dense in  $H_0^3$ , an element  $\hat{\phi}$  may be chosen from  $I$  so that the quantities  $|z^N(t; \phi, q) - z^N(t; \hat{\phi}, q)|$  and  $|z(t; \phi, q) - z(t; \hat{\phi}, q)|$  are as small as desired (uniformly in  $t$ ,  $q$ , and  $N$ ; see Theorems 2.1 and 3.1). Therefore, for any  $t \in [t_1, t_r]$ , we find that

$$\begin{aligned} & |z^N(t; \phi, q^N) - z(t; \phi, \tilde{q})| \\ & \leq |z^N(t; \phi, q^N) - z^N(t; \hat{\phi}, q^N)| \\ & \quad + |z^N(t; \hat{\phi}, q^N) - z(t; \hat{\phi}, \tilde{q})| \\ & \quad + |z(t; \hat{\phi}, \tilde{q}) - z(t; \phi, \tilde{q})| \end{aligned}$$

will be arbitrarily small for  $N$  sufficiently large. The convergence result thus obtains.

Remark 3.1. If the perturbing function  $f$  is independent of  $q$ , it is useful to note that we may relax the spatial differentiability requirements on  $f$  (given in (H1)) in much the same way that this was done for  $\phi$  in Theorem 3.4 above. That is, we may replace (H1)-(H3) by (H1)' and (H2)', given below, and obtain the initial convergence results (Theorem 3.3) for  $\{\phi, f\}$  in a smooth but dense subset of  $H_0^3 \times L_2(U)$ ; as before, the additional smoothness is needed to guarantee that the corresponding solution  $z(t; \phi, f, q)$  belongs to  $\mathcal{Z}$  for  $t \in [t_1, t_r]$ . Under the new hypotheses on  $f$ , existence and uniqueness of solutions to the original parabolic equation are still assured.

(H1)' The perturbation function  $(t, x) \mapsto f(t, x)$  and its derivative  $\frac{\partial f}{\partial t}$  are uniformly Hölder continuous on  $U$  with exponent in  $(0, 1)$ .

(H2)' The function  $f$  satisfies  $f(0,0) = f(0,1) = 0$ .

We note, however, that a price must be paid for this formulation of the problem: When  $q_2 \neq 0$  or  $q_3 \neq 0$ , nonhomogeneous boundary conditions can no longer be allowed since the transformation to homogeneous boundary conditions (see (2.5), (2.6)) necessarily generates a  $q$ -dependent perturbing function.

We should also remark on another technical aspect of the above presentation. The reader might be curious as to why we choose the first sampling time  $t_1$  strictly positive and carry out the convergence proofs (see (3.1), (3.2) and Theorem 3.4) on  $[t_1, T]$  instead of the (perhaps) more natural interval  $[0, T]$ . This is a purely technical matter, since if we take  $t_1 = 0$  the establishment of the fundamental results of Lemma 3.3 becomes more delicate. In particular, we can then no longer use Corollary 1 of [18, p. 78] as we did in the proof of that lemma. However, if we make further smoothness assumptions on the data of our problem (e.g., the coefficients, initial data, nonhomogeneous perturbing function  $f$ ), we can instead invoke Corollary 2 of [18, p. 78] to obtain the desired bounds and convergence results on  $[0, T] \times [0, 1]$  in place of  $[t_1, T] \times [0, 1]$  where  $t_1 > 0$ . In our calculations in section 4 below, we actually approximate the functional coefficients on  $[0, T]$  and exhibit the convergence in this case.

The smoothness assumptions that we have assumed on the coefficients are reasonable unless one is dealing with problems in which the coefficients have jump discontinuities. Our methods also perform well in such situations (this comment is based on use of our techniques in numerical calculations for other classes of estimation problems), but the above theory does not extend in a straightforward manner. Rather, one can use a weak formulation of the system (2.1)-(2.3) (e.g., see [10]) to develop a convergence theory in this case.

To this point we have focused on the convergence of solutions  $z^N$  (of (3.3)) to the solution  $z$  (of (3.1)) once the convergence of any sequence of parameters has been assured. In reality however, we have yet to determine whether any sequence of solutions  $\{\bar{q}^N\}$  of the approximating problems is in fact convergent; even then we have no guarantee that the limiting function  $\bar{q}$  is indeed a solution to the original parameter estimation problem. Our next result, (similar in spirit to that found in [4], [9], [13]), addresses this question and indicates when an approximate identification problem may be used to compute numerical solutions for the original problem.

Theorem 3.5. Let  $\{\bar{q}^N\}$  be given, where each  $\bar{q}^N$  is a solution to the approximate parameter identification problem for (3.3), (3.4). Then there exists  $\bar{q} \in Q$  and a subsequence  $\{\bar{q}^{N_k}\}$  such that  $\bar{q}^{N_k} \rightarrow \bar{q}$  and  $\bar{q}$  is a solution to the original estimation problem for (2.9), (2.12).

Proof: Since  $Q$  is compact, convergence of a subsequence  $\{\bar{q}^{N_k}\}$  to some  $\bar{q}$  in  $Q$  is ensured. In fact, it is easy to see that  $\bar{q}$  is a solution to the original parameter estimation problem. From (2.12),

$$\begin{aligned}
 J(\bar{q}) &= \sum_{i=1}^r |\hat{y}_i - c(t_i, \bar{q})z(t_i; \bar{q})|^2 \\
 &= \lim_{N_k \rightarrow \infty} \sum_{i=1}^r |\hat{y}_i - c(t_i, \bar{q}^{N_k})z^{N_k}(t_i; \bar{q}^{N_k})|^2 \\
 &= \lim_{N_k \rightarrow \infty} J^{N_k}(\bar{q}^{N_k}) \\
 &\leq \lim_{N_k \rightarrow \infty} J^{N_k}(q)
 \end{aligned}$$

for any  $q \in Q$ . But Theorem 3.4 is also valid with the constant sequence  $\{q\}$ , so that  $z^N(t; q) \rightarrow z(t; q)$  uniformly in  $t \in [t_1, t_r]$ ; we are thus guaranteed that

$$\lim_{N_k \rightarrow \infty} J^{N_k}(q) = J(q)$$

so that  $J(\bar{q}) \leq J(q)$  for any  $q \in Q$ .

In the discussions thus far, our problems have been formulated in terms of iterations and searches in the parameter function space  $Q$ . Of course, we cannot realize such searches on a computer. Indeed we must have for the elements in  $Q$  some type of representation amenable to implementation. One possibility (see [12]) is to assume an a priori functional representation (e.g., polynomials of degree  $\leq k$  with coefficients ranging over some given set) so that the parameters sought and convergence argued actually involve finitely many constants in some fixed subsets of Euclidean space. For this approach one must have an idea of the form (shape) of the unknown functional coefficients. In this event the above-developed theory obviously suffices to establish convergence results and an implementable scheme. However our theoretical framework is, in reality, much more general and can be employed to develop methods where one actually searches for the shape of functional coefficients by seeking functional approximations (say in the space of linear or cubic splines). We do this in the examples of section 4 below. To illustrate how the above theory can be applicable in this situation (we recall that all the results are given for  $Q$  compact in the  $L_2$  sense and that the continuous dependence of  $z$  and  $J$  on  $q$  is in the  $L_2$  norm), we first consider the case where one uses piecewise linear

spline approximations to functions in  $Q$  (which is natural if  $Q$  is compact in the  $C$  or supremum norm topology).

We assume that  $Q \subset C$  is compact in the  $C$  topology and let  $L^t(M_1)$  and  $L^x(M_2)$  denote the spaces of piecewise linear splines (see [27, p. 11]) corresponding to equal partitions of  $[t_1, T]$  and  $[0, 1]$  of mesh size  $\frac{T-t_1}{M_1}$  and  $\frac{1}{M_2}$ , respectively. That is, we use the piecewise linear splines with knots  $t_k = t_1 + (k-1)((T-t_1)/M_1)$ ,  $k = 1, 2, \dots, M_1+1$ , and  $x_m = (m-1)/M_2$ ,  $m = 1, 2, \dots, M_2+1$ . We denote the corresponding 2-dimensional interpolating linear spline operator by  $I^M$  where  $M = (M_1, M_2)$ . Thus if  $q$  is continuous on  $[t_1, T] \times [0, 1]$ ,

$$(I^M q)(t, x) = \sum_{k=1}^{M_1+1} \sum_{m=1}^{M_2+1} q(t_k, x_m) \beta_k(t) \rho_m(x)$$

where  $\beta_k = \beta_k^{M_1}$  and  $\rho_m = \rho_m^{M_2}$  are the appropriately normalized (depending of course on the partition mesh) usual "patch" function piecewise linear basis elements [27, p. 11] defined on the intervals  $[t_1, T]$  and  $[0, 1]$ , respectively. Clearly the mapping  $I^M: Q \rightarrow C$  is continuous (in the  $C$  topology on  $Q$ ) and hence  $Q^M \equiv I^M(Q)$  is compact in  $C$ . Since any  $q = (q_1, q_2, \dots, q_n)$  in  $Q^M$  can be written as  $q = I^M(\tilde{q})$  for some  $\tilde{q} \in Q$ , it follows that  $Q^M$  has the representation

$$(3.17) \quad Q^M = \left\{ q: [t_1, T] \times [0, 1] \rightarrow R^n \mid q_i = \sum_k \sum_m \delta_{ikm} \beta_k \rho_m, \delta_{ikm} \in \Delta_{ikm} \right\}$$

where the  $\Delta_{ikm}$  are appropriately chosen compact subsets of  $R^1$ .

We then carry out the minimization procedure (for  $J^N$ ) described earlier in this paper over the function set  $Q^M$ , obtaining, for each state approximation index  $N$ , a best parameter function  $\bar{q}^N(M)$  in  $Q^M$ . Due to the compactness of  $Q^M$ , we can extract a subsequence (we relabel to avoid subsequence notation) converging to some limit function  $\bar{q}(M)$  in  $Q^M$ , i.e.,  $\bar{q}_i(M) = \lim_{N \rightarrow \infty} \bar{q}_i^N(M)$ ,

$i = 1, \dots, n$ . From our earlier discussions (Theorem 3.5),  $\bar{q}(M)$  provides a minimum for  $J$  over  $Q^M$ . From the definition of  $Q^M$ , it follows there exists  $\hat{q}(M) \in Q$  such that  $\bar{q}(M) = I^M(\hat{q}(M))$  for each  $M$ . From the compactness of  $Q$ , we can extract a subsequence  $\hat{q}(M^j)$  such that  $\hat{q}(M^j)$  converges (in  $C$  norm) as  $M^j \rightarrow \infty$  (recall  $M = (M_1, M_2)$  and hence by  $M^j \rightarrow \infty$  we shall mean  $M_1^j \rightarrow \infty$  and  $M_2^j \rightarrow \infty$ ) to some element  $q^*$  in  $Q$ .

To argue that  $q^*$  is a solution to our original problem of minimizing  $J$  over  $Q$ , we need further assumptions. Specifically we assume  $Q \subset H^2$  with the quantities  $|\partial_x^2 q|$ ,  $|\partial_t^2 q|$ ,  $|D_x D_t q|$  uniformly bounded as  $q$  ranges over  $Q$ . Then we also find that  $I^{M^j}(\hat{q}(M^j)) \rightarrow q^*$  in the  $L_2$  topology since

$$(3.18) \quad |I^{M^j}(\hat{q}(M^j)) - q^*| \leq |I^{M^j}(\hat{q}(M^j)) - \hat{q}(M^j)| + |\hat{q}(M^j) - q^*|$$

$$\leq \frac{C_0}{(M_1^j)(M_2^j)} + |\hat{q}(M^j) - q^*|$$

and this last expression (the first term of which follows from a minor modification of Theorem 2.7 of [27, p. 19]) approaches zero as  $M^j \rightarrow \infty$ .

Recalling that  $J(\bar{q}(M)) \leq J(q)$  for all  $q \in Q^M$ , and, given the fact that  $Q^M = I^M(Q)$ , thus

$$(3.19) \quad J(\bar{q}(M)) \leq J(I^M(q)) \quad \text{for all } q \in Q,$$

we next observe that the same basic spline result used in (3.18) yields

$I^M(q) \rightarrow q$  for any  $q \in Q$ . Furthermore, since  $\bar{q}(M) = I^M(\hat{q}(M))$  for all  $M$  and  $I^{M^j}(\hat{q}(M^j)) \rightarrow q^*$ , we may use the continuity of  $J$  (in the  $L_2$  sense) to take limits in

$$J(I^{M^j}(\hat{q}(M^j))) \leq J(I^{M^j}(q)), \quad q \in Q,$$

to obtain

$$J(q^*) \leq J(q) \quad \text{for all } q \in Q.$$

We thus find that  $q^* = \lim_{M^j \rightarrow \infty} \hat{q}(M^j) = \lim_{M^j \rightarrow \infty} I^{M^j}(\hat{q}(M^j)) = \lim_{M^j \rightarrow \infty} \bar{q}(M^j) =$

$\lim_{M^j \rightarrow \infty} \lim_{N_k \rightarrow \infty} \bar{q}^{N_k}(M^j)$  provides a minimum for  $J$  over  $Q$ . We summarize our findings

in the formal statement:

**Theorem 3.6.** Suppose  $Q \subset H^2$  with  $|D_x^2 q|$ ,  $|D_t^2 q|$ ,  $|D_t D_x q|$  uniformly bounded for  $q \in Q$ . Further assume that  $Q$  is compact in its  $C$  topology and let  $Q^M = I^M(Q)$  denote the linear spline approximation sets as given in (3.17). Let  $\bar{q}^N(M)$  be a solution obtained from minimizing  $J^N$  (see (3.4)) over  $Q^M$ . Then there exists  $q^*$  in  $Q$  minimizing  $J$  over  $Q$  and a subsequence  $\bar{q}^{N_k}(M^j)$  with  $q^* = \lim_{M^j \rightarrow \infty} (\lim_{N_k \rightarrow \infty} \bar{q}^{N_k}(M^j))$ .

We next consider approximating the parameter functions with bicubic elements. That is, we assume the basis elements  $\beta_k$  and  $\rho_m$  in (3.17) are those for  $S^t(M_1)$  and  $S^x(M_2)$ , the cubic splines [27, p. 44, 48, 49] on  $[t_1, T]$  and  $[0, 1]$ , respectively. The corresponding bicubic interpolating map  $I^M$  is continuous in the  $C^2$  topology on  $Q$  (the interpolation map involves functional values of  $q$  at interior grid points of  $[t_1, T] \times [0, T]$ , values of  $D_t q$ ,  $D_x q$  at lateral boundaries, and those of  $D_t D_x q$  at the corners -- see [27, p. 49, 50]). If we assume that  $Q$  is  $C^2$  compact, we again can obtain a representation for  $Q^M = I^M(Q)$  of the form (3.17) where the coefficients range over compact sets in  $R^1$ . To make arguments analogous to those involving (3.18), (3.19), we need only to further assume  $Q \subset H^4$  with  $|D_x^4 q|$ ,  $|D_t^4 q|$ ,  $|D_t^2 D_x^2 q|$  uniformly

bounded for  $q \in Q$  and employ Theorem 4.9 (which holds with  $PC^{4,2}$  replaced by  $H^4$ ) of [27, p. 60]. The following corollary to the above results is thus obtained.

**Corollary 3.7.** Suppose  $Q \subset H^4$  is compact in the  $C^2$  topology with  $|D_x^4 q|$ ,  $|D_t^4 q|$ ,  $|D_t^2 D_x^2 q|$  uniformly bounded for  $q \in Q$ . Let  $Q^M = I^M(Q)$  denote the bicubic spline approximations to  $Q$  as defined above. Then the conclusions of Theorem 3.6 are also valid in this case.

If the parameter functions are separable, i.e.,  $q_i(t, x) = h_i(t)c_i(x)$ , we can relax the assumptions in the above theorem and corollary. For example suppose  $Q_1 \subset \{h: [t_1, T] \rightarrow R^n\}$  and  $Q_2 \subset \{c: [0, 1] \rightarrow R^n\}$  are given subsets of  $H^1$  with both  $Q_1, Q_2$  compact in their respective  $C$  topologies and let  $Q = Q_1 \otimes Q_2$ . That is,  $Q = \{q = h \otimes c \mid h \in Q_1, c \in Q_2\}$  so that the components of  $q \in Q$  are given by  $q_i(t, x) = h_i(t)c_i(x)$ ,  $i = 1, 2, \dots, n$ . We further assume that  $|Dh|_2$ ,  $|Dc|_2$  are uniformly bounded in  $h \in Q_1, c \in Q_2$ .

Let  $I_t^{M_1}$  and  $I_x^{M_2}$  denote the piecewise linear interpolating splines [27, p. 11] on  $[t_1, T]$  and  $[0, 1]$  corresponding to mesh sizes  $\frac{T-t_1}{M_1}$  and  $1/M_2$ , respectively. Then  $I_t^{M_1}$  and  $I_x^{M_2}$  are continuous from  $Q_1$  and  $Q_2$  (with their  $C$  topologies) to  $L^t(M_1)$  and  $L^x(M_2)$ , respectively, and both  $Q_1^{M_1} \equiv I_t^{M_1}(Q_1)$  and  $Q_2^{M_2} \equiv I_x^{M_2}(Q_2)$  are compact with representations

$$Q_1^{M_1} = \left\{ h: [t_1, T] \rightarrow R^n \mid h_i(t) = \sum_{k=1}^{M_1+1} \alpha_{ik} \beta_k(t), \quad \alpha_{ik} \in \alpha_{ik} \right\}$$

and

$$Q_2^{M_2} = \left\{ c: [0, 1] \rightarrow R^n \mid c_i(x) = \sum_{m=1}^{M_2+1} \gamma_{im} \rho_m(x), \quad \gamma_{im} \in \Gamma_{im} \right\}$$

where  $\alpha_{ik}, \Gamma_{im}$  are compact subsets of  $R^1$ .



We then can carry out the minimization (for each  $N$ ) of  $J^N$  over  $Q^M \equiv Q_1^{M_1} \otimes Q_2^{M_2}$ , obtaining minimizers  $\bar{q}^N(M) = \bar{h}^N(M_1) \otimes \bar{c}^N(M_2)$ . The compactness of  $Q_1^{M_1}$  and  $Q_2^{M_2}$  imply the existence of convergent subsequences  $\{\bar{h}^{N_k}(M_1)\}$ ,  $\{\bar{c}^{N_k}(M_2)\}$  with  $\bar{h}^{N_k}(M_1) \rightarrow \bar{h}(M_1)$ ,  $\bar{c}^{N_k}(M_2) \rightarrow \bar{c}(M_2)$  where  $\bar{q}(M) \equiv \bar{h}(M_1) \otimes \bar{c}(M_2) \in Q^M$ . It follows that there exist  $\hat{h}(M_1)$ ,  $\hat{c}(M_2)$  in  $Q_1$ ,  $Q_2$  such that  $\bar{h}(M_1) = I_t^{M_1}(\hat{h}(M_1))$ ,  $\bar{c}(M_2) = I_x^{M_2}(\hat{c}(M_2))$ . Since  $Q_1$ ,  $Q_2$  are compact, we may obtain convergent subsequences of  $\{\hat{h}(M_1)\}_{M_1=1}^\infty$ ,  $\{\hat{c}(M_2)\}_{M_2=1}^\infty$  (relabeling if necessary, we again call them  $\{\hat{h}(M_1)\}$ ,  $\{\hat{c}(M_2)\}$ ) converging as  $M_1 \rightarrow \infty$ ,  $M_2 \rightarrow \infty$  to  $h^*$ ,  $c^*$  in  $Q_1$ ,  $Q_2$  respectively. It follows that (here we distinguish between the  $L_2$  and  $L_\infty$  norms)

$$\begin{aligned}
& |I_t^{M_1}(\hat{h}(M_1)) \otimes I_x^{M_2}(\hat{c}(M_2)) - h^* \otimes c^*|_2 \\
& \leq |I_t^{M_1}(\hat{h}(M_1)) \otimes I_x^{M_2}(\hat{c}(M_2)) - \hat{h}(M_1) \otimes \hat{c}(M_2)|_2 + |\hat{h}(M_1) \otimes \hat{c}(M_2) - h^* \otimes c^*|_2 \\
& \leq |I_t^{M_1}(\hat{h}(M_1)) \otimes [I_x^{M_2}(\hat{c}(M_2)) - \hat{c}(M_2)]|_2 \\
& \quad + |[I_t^{M_1}(\hat{h}(M_1)) - \hat{h}(M_1)] \otimes \hat{c}(M_2)|_2 + |\hat{h}(M_1) \otimes \hat{c}(M_2) - h^* \otimes c^*|_2 \\
& \leq K |I_t^{M_1}(\hat{h}(M_1))|_\infty |I_x^{M_2}(\hat{c}(M_2)) - \hat{c}(M_2)|_2 \\
& \quad + K |\hat{c}(M_2)|_\infty |I_t^{M_1}(\hat{h}(M_1)) - \hat{h}(M_1)|_2 + |\hat{h}(M_1) \otimes \hat{c}(M_2) - h^* \otimes c^*|_2 \\
& \leq (M/M_2) \sup_{c \in Q_2} |Dc|_2 + (M(T-t_1)/M_1) \sup_{h \in Q_1} |Dh|_2 \\
& \quad + |\hat{h}(M_1) \otimes \hat{c}(M_2) - h^* \otimes c^*|_2 \\
& \rightarrow 0 \quad \text{as } M_1, M_2 \rightarrow \infty,
\end{aligned}$$

where the first two terms in the last estimate follow from Theorem 24 of [27, p. 16].

From the above one can conclude (the arguments are similar to those following (3.18)) that  $q^* = h^* \otimes c^*$  is a solution of the original problem of minimizing  $J$  over  $Q$ . We thus have:

**Theorem 3.8.** Suppose  $Q = Q_1 \otimes Q_2$  with  $Q_i \subset H^1$ ,  $Q_i$  compact in its  $C$  topology with  $|Dh|$ ,  $|Dc|$  uniformly bounded for  $h \in Q_1$ ,  $c \in Q_2$ . Let  $Q^M = Q_1^{M_1} \otimes Q_2^{M_2}$  be the (linear) spline approximation to  $Q$  as defined above and let  $\bar{q}^{N(M)} = \bar{h}^N(M_1) \otimes \bar{c}^N(M_2)$  be a solution to the problem of minimizing  $J^N$  over  $Q^M$ . Then there exists  $q^* = h^* \otimes c^*$  in  $Q$  which provides a minimum for  $J$  over  $Q$  and a subsequence  $\bar{q}^{N_k(M_j)}$  such that  $q^* = h^* \otimes c^* = \lim_{\substack{M_1^j \rightarrow \infty, \\ M_2^j \rightarrow \infty}} \left( \lim_{N_k \rightarrow \infty} \bar{h}^{N_k}(M_1^j) \otimes \bar{c}^{N_k}(M_2^j) \right)$ .

There is an obvious corollary to this theorem involving use of cubic splines. If  $Q = Q_1 \otimes Q_2$  and we wish to use the cubic splines  $S^t(M_1)$  and  $S^x(M_2)$  to approximate the sets  $Q_1$  and  $Q_2$ , respectively, the conclusions of Theorem 3.8 are valid under the assumptions that  $Q_i \subset H^2$ ,  $Q_i$  compact in its  $C^1$  topology with  $|D^2h|$ ,  $|D^2c|$  uniformly bounded for  $h \in Q_1$ ,  $c \in Q_2$  (compare with the assumptions of Corollary 3.7). Finally one can also wish (in the separable  $Q = Q_1 \otimes Q_2$  case) to approximate one parameter set (say  $Q_1$ ) by linear spline elements ( $L^t(M_1)$ ) while approximating the other,  $Q_2$ , by cubic elements ( $S^x(M_2)$ ) (see the examples in section 4). Obvious analogues of the above convergence results can be easily given in these cases also.

#### §4 Numerical results

In this section we present our numerical findings for a number of representative parameter estimation problems, including an example that illustrates how our spline-based methods can be used to identify variable diffusion and convection parameters in a dispersion model. The goal of our efforts was to establish the effectiveness of these methods as they are used to determine a variety of parameters that depend on time and/or spatial variables, and to observe convergence properties in several different examples. To this end, we developed a Fortran software package (a modification of one created by Dr. James Crowley when he was a student at Brown University) to identify parameters in the  $N^{\text{th}}$  approximate ODE system (3.11); all test computations were carried out on the CDC 6600 at Southern Methodist University.

The numerical examples that appear in this section were formulated in the following manner: "True" parameter functions  $\bar{q} = (\bar{q}_1, \bar{q}_2, \bar{q}_3)$  and a true solution  $\bar{u}(t,x)$  were chosen for each example a priori. (In each case,  $\bar{u}(t,0) = \bar{u}(t,1) = 0$ , although only Example 4.1 satisfies the hypothesis that the initial data  $\phi$  lie in  $H_0^3$ . Indeed, it is not surprising that the methods under investigation perform admirably when applied to examples that satisfy weaker assumptions than those we used in arguing theoretical convergence.) An  $r \times (s-1)$  grid of sample data points  $\hat{y}_{ij}$  was determined by setting  $\hat{y}_{ij} = \bar{u}(t_i, x_j)$  (with random noise added in Example 4.1) where  $t_i = (i-1)T/r$ ,  $i = 1, \dots, r$ , and  $x_j = j/s$ ,  $j = 1, \dots, s-1$ . The estimation problem then becomes that of determining  $\bar{q} \in Q$  (and  $u(\bar{q})$ ) that minimizes

$$J(q) = \sum_{i,j} |\hat{y}_{ij} - u(t_i, x_j; q)|^2$$

where  $u$  satisfies (2.1)-(2.3); for each example,  $\phi$  and  $f$  were given at the outset by  $\phi(x) = \bar{u}(0,x)$  and

$$f(t,x) = \frac{\partial \bar{u}}{\partial t} - \bar{q}_1(t,x) \frac{\partial^2 \bar{u}}{\partial x^2} - \bar{q}_2(t,x) \frac{\partial \bar{u}}{\partial x} - \bar{q}_3(t,x) \bar{u}(t,x).$$

We remark here that the cost functional  $J$  defined above is not even a special case of the distributed least squares fit-to-data functional given in (2.4). We could have, of course, interpolated our data  $\{\hat{y}_{ij}\}$  and used (2.4); this would have kept us in the framework developed above. We didn't do this since it has been our experience that one actually obtains a much stronger convergence (pointwise in  $x$ ) for  $z^N(t;q) = u^N(t, \cdot, q)$  than the norm convergence that is usually guaranteed a priori by the theory (for cases where one can establish the stronger convergence see Lemma 2.4 and Theorem 2.1 of [7]). In addition, we have in our numerical tests violated the assumption that the first sample time,  $t_1$ , be strictly positive ( $t_1 = 0$  for all of our examples). No real problems are posed by these discrepancies however: As was noted earlier, this particular restriction may be relaxed if we are willing to assume additional smoothness on the coefficients  $q$ . Continuity requirements of this sort are certainly met in the test examples chosen here.

Several different finite-dimensional representations for the functional parameters were discussed in detail in section 3. We assume throughout this section that  $q_i(t,x) = h_i(t)c_i(x)$  and, for a given  $N$ , attempt to identify "optimal" approximations for  $h_i$  in  $L^t(M_1)$  or  $S^t(M_1)$  and  $c_i$  in  $L^x(M_2)$  or  $S^x(M_2)$ ,  $i = 1,2,3$ ; that is, given initial guesses for  $\alpha_{ik}$  and  $\gamma_{im}$ , we determine  $\bar{\alpha}_{ik}^N$  and  $\bar{\gamma}_{im}^N$ ,  $k = 1, \dots, K_1(M_1)$ ,  $m = 1, \dots, K_2(M_2)$ , so that

$$h_i^N(t) = \sum_{k=1}^{K_1} \bar{\alpha}_{ik}^N \beta_k(t)$$

and

$$\bar{c}_i^N(x) = \sum_{m=1}^{K_2} \bar{\gamma}_{im}^N \rho_m(x)$$

are "optimal" in the sense described in previous sections. For each example, we take  $M_1$  and  $M_2$  fixed; thus there should be no confusion in writing  $\bar{\alpha}_{ik}^N$  and  $\bar{\gamma}_{im}^N$  throughout, instead of the intended meaning,  $\bar{\alpha}_{ik}^N(M_1)$  and  $\bar{\gamma}_{im}^N(M_2)$ . We remark here that this choice of approximation for  $h_i$ ,  $c_i$  simplifies the effort required to implement the approximating parameter estimation problems. Because standard parameter identification packages require that (3.11), the system in  $w^N$ , be solved for each updated value of  $q$ , the inner product matrices  $K_i^N$ ,  $i = 1, 2, 3$ , need to be recomputed for each  $q$ -iterate. This is a simple matter given the representations chosen here; for example, the  $(i, j)$ -entry of  $K_1^N$  becomes

$$h_i(t) \langle c_j D^2 B_j^N, B_i^N \rangle = \left( \sum_{k=1}^{K_1} \alpha_{ik} \beta_k(t) \right) \sum_{m=1}^{K_2} \gamma_{jm} \langle \rho_m D^2 B_j^N, B_i^N \rangle$$

so that the inner products need to be computed only once (prior to the iterative process) and simply combined appropriately as  $\alpha_{ik}$  and  $\gamma_{jm}$  are updated.

Our experience with numerous numerical examples has indicated that greater accuracy is required for the spline representation for  $c_i$  than for  $h_i$ , which is not surprising since  $c_i$  is involved in calculating the inner products for  $K_1^N$ , etc. For this reason, we chose  $L^t(M_1)$  for  $h_i$  and  $S^x(M_2)$  for  $c_i$  in the examples presented here, except for Example 4.3 where  $L^x(M_2)$  is used for  $c_i$  as well. The choice of  $M_1$  and  $M_2$  is clearly problem-dependent, especially when the time interval  $[0, T]$  is very large; in what follows we pick  $M_1$  and  $M_2$

so that both  $L^t(M_1)$  and  $S^X(M_2)$  have exactly four basis elements, a number large enough to ensure reasonably accurate approximations for  $h_i$  and  $c_i$  yet small enough to keep the number of unknowns ( $\alpha_{ik}, \gamma_{im}$ ;  $i = 1, 2, 3$ ;  $k = 1, \dots, K_1$ ;  $m = 1, \dots, K_2$ ) at a manageable level. We therefore take  $M_1 = 3$  and  $M_2 = 1$ , except in Example 4.2, where the four basis elements for  $S^X(M_2)$  are modified to satisfy homogeneous boundary conditions (and thus  $M_2 = 3$  must be taken).

For given values of  $N$ ,  $M_1$ , and  $M_2$ , we used ZXSSQ, the IMSL version of the Levenberg-Marquardt algorithm, to iteratively determine the desired parameters. Our experience with this package has been relatively good (it is easily implemented and usually performs well with default values for several of the required input variables) so long as we did not need to estimate more than a combined total of 7 or 8 unknown coefficients in the approximation for  $h_i$  and  $c_i$ . The package tends to fail in attempts to estimate a larger number of parameters and this may be due to the fact that ZXSSQ computes all needed gradients using a finite difference scheme (although preliminary testing of MINPACK's version of the Levenberg-Marquardt scheme, LMSTR1, with more accurate user-supplied gradients, has not indicated that this is necessarily the sole source of the difficulty). It is more likely that a large number of unknown parameters is associated with an excessive number of degrees of freedom in the problem, which manifests itself in the inability of the iterative scheme to converge at all to  $\bar{q}^N(M)$  for  $N$  and  $M$  fixed.

As can be expected, increasing the number of unknowns also increases the CP time required, as well as the number of requisite iterations on  $q$ . It was also our experience that it was far more difficult to identify  $c_i$  than  $h_i$ , possibly due to the fact that  $c_i$  always appears in integrated form (in the inner product matrices) which suggests that the solution  $w^N$  to (3.11)

is less sensitive to small changes in  $c_i$  than it is with respect to changes in  $h_i$ . In such examples the parameter estimation process was frequently quite expensive (CP time for  $N=3$  problems with 6-8 unknown coefficients for  $h_i$  and  $c_i$  often exceeded 1000 seconds; in contrast, it took only 345 CP seconds to accurately identify the 8 unknowns in Example 4.1. where parameters did not depend on the spatial variable). Even with fewer unknowns, these parameter estimation problems are generally more expensive (137 CP seconds for Example 4.1(a);  $N=2$ ) than those for many other distributed systems (see [9], [10]) because the approximating ODE systems for these parabolic PDEs tend to be quite stiff, requiring more costly solution schemes (for example, IMSL's DGEAR, which is what we used in our computations).

We turn now to several numerical examples that are representative of our findings. In example 4.1 and 4.2 we display  $\bar{q}^N = \bar{q}^N(M)$  for  $N = 2, 4, 8$ , and 16, (values of  $M_1$  or  $M_2$  for  $M$  are fixed throughout, as was previously indicated) to demonstrate how quickly  $\bar{q}^N$  approaches  $\bar{q}$ ; in fact, convergence is so rapid in these examples that we present only  $\bar{q}^3$  for the remaining examples.

#### Example 4.1

We consider the system

$$\begin{cases} u_t = q_1(t)u_{xx} + q_2(t)u_x + f(t,x), & 0 < x < 1, \quad 0 < t \leq 1, \\ u(0,x) = 0 \\ u(t,0) = u(t,1) = 0. \end{cases}$$

A  $9 \times 3$  grid of sample data points was generated from the "true" values of the solution and parameters,  $\bar{u}(t,x) = 100x(1-x)(x+4)\sin\pi t$ ,  $\bar{q}_1(t) = 8t+1$ , and  $\bar{q}_2(t) = -2t+4$ . "True" coefficient values for the representations

$q_1(t) = \sum_{k=1}^4 \alpha_{1k} \beta_k(t)$  and  $q_2(t) = \sum_{k=1}^4 \alpha_{2k} \beta_k(t)$  are then given by  $\bar{\alpha}_{11} = 1$ ,  
 $\bar{\alpha}_{12} = 3\frac{2}{3}$ ,  $\bar{\alpha}_{13} = 6\frac{1}{3}$ ,  $\bar{\alpha}_{14} = 9$ ,  $\bar{\alpha}_{21} = 4$ ,  $\bar{\alpha}_{22} = 3\frac{1}{3}$ ,  $\bar{\alpha}_{23} = 2\frac{2}{3}$ ,  $\bar{\alpha}_{24} = 2$   
 (in each case,  $\bar{\alpha}_{ik} = \bar{\alpha}_{ik}(M)$ ,  $i = 1, 2$ ;  $k = 1, \dots, 4$ ). Several different estimation problems were investigated.

- (a) We seek to estimate  $q_1$  with  $q_2 = \bar{q}_2$  given. For our initial guess we take  $q_1 \equiv .001$ ; that is,  $\alpha_{1k} = .001$ ,  $k = 1, \dots, 4$ .

N	$\bar{\alpha}_{11}^N$	$\bar{\alpha}_{12}^N$	$\bar{\alpha}_{13}^N$	$\bar{\alpha}_{14}^N$
2	0.998581	3.629449	6.250314	8.880572
4	0.999974	3.666598	6.333214	8.999806
8	0.999975	3.666598	6.333214	8.999806
16	0.999974	3.666598	6.333214	8.999806

- (b) We repeat the computations in (a) except that we corrupt the "data" with random noise (varying between  $-1$  and  $+1$ ).

N	$\bar{\alpha}_{11}^N$	$\bar{\alpha}_{12}^N$	$\bar{\alpha}_{13}^N$	$\bar{\alpha}_{14}^N$
2	1.044241	3.605704	6.282895	8.932719
4	1.046339	3.642512	6.366286	9.051935
8	1.045438	3.640817	6.368787	9.049063
16	1.041110	3.643830	6.366950	9.050610

- (c) We estimate both  $q_1$  and  $q_2$ , using start-up values of  $q_1 \equiv 5.0$  and  $q_2 \equiv 1.5$  ( $\alpha_{1k} = 5.0$ ,  $\alpha_{2k} = 1.5$ ,  $k = 1, \dots, 4$ ). The results are reported in Table 4.1.



Table 4.1

N	$-\alpha_{11}^N$	$-\alpha_{12}^N$	$-\alpha_{13}^N$	$-\alpha_{14}^N$	$-\alpha_{21}^N$	$-\alpha_{22}^N$	$-\alpha_{23}^N$	$-\alpha_{24}^N$
2	1.000889	3.624683	6.236901	8.858657	3.831947	2.835039	1.861841	0.864159
4	0.999976	3.666598	6.333214	8.999806	3.999931	3.333287	2.666577	2.000122
8	0.999975	3.666598	6.333214	8.999806	3.999907	3.333295	2.666590	2.000039
16	0.999977	3.666600	6.333210	8.999790	3.999860	3.333310	2.666570	2.000180

Table 4.2

N	$-\alpha_{11}^N$	$-\alpha_{12}^N$	$-\alpha_{13}^N$	$-\alpha_{14}^N$	$-\alpha_{21}^N$	$-\alpha_{22}^N$	$-\alpha_{23}^N$	$-\alpha_{24}^N$
2	1.043473	3.601573	6.269343	8.893955	3.599734	2.852122	1.863598	0.000000
4	1.049475	3.642015	6.366801	9.041126	3.713071	3.401195	2.680427	0.527317
8	1.053841	3.641693	6.366734	9.041618	3.774700	3.357572	2.709742	0.541403
16	1.054040	3.639160	6.373950	9.034400	3.784480	3.455270	2.599440	0.843230

- (d) We repeat the calculations in (c) except we corrupt the data with random noise as in (b). Table 4.2 contains the outcome of this investigation. The addition of random noise in this case yields satisfactory estimates for all coefficients except  $\alpha_{24}$ , which appears to be converging to a value far from  $\bar{\alpha}_{24} = 2$ . We were able to determine however that  $J(\bar{q}^{16}) < J(\bar{q})$  for this example so that the parameters  $q_1$  and  $q_2$  that provide the best fit to the new (noisy) data are not merely slight deviations from the parameters that generated the original (noise-free) data.

#### Example 4.2

We consider

$$\begin{cases} u_t = q_1(x)u_{xx} + q_2(x)u_x + f(t,x), & 0 < x < 1, \quad 0 < t \leq 2, \\ u(0,x) = -20(x^2 - x) \\ u(t,0) = u(t,1) = 0 \end{cases}$$

with  $\bar{q}_1(x) = x - x^2$ ,  $\bar{q}_2(x) = 8x - 8x^2$  and true solution  $\bar{u}(t,x) = -10(x^2 - x)(t^2 + 4t + 2)$ .

A  $9 \times 3$  grid of sample data was used to search for estimates  $\bar{q}_1^N$  and  $\bar{q}_2^N$  in

$$S_0^X(3) = \left\{ \sum_{m=1}^4 \gamma_{im} \rho_m \mid \rho_m \text{ is a cubic B-spline modified so that } \rho_m(0) = \rho_m(1) = 0, \right.$$

$m = 1, \dots, 4 \left. \right\}$  (the spline elements  $\rho_m$  are defined exactly the same as  $B_m^M$  for  $M = 3$ , where  $B_m^M$  was given in section 3). We compare our computed values with those corresponding to the projections  $P^M q_i = P^3 q_i$  which have the coefficients  $\bar{\gamma}_{11} = 0.01698$ ,  $\bar{\gamma}_{12} = 0.04321$ ,  $\bar{\gamma}_{13} = 0.04321$ ,  $\bar{\gamma}_{14} = 0.01698$ , and  $\bar{\gamma}_{21} = 0.13580$ ,  $\bar{\gamma}_{22} = 0.34568$ ,  $\bar{\gamma}_{23} = 0.34568$ ,  $\bar{\gamma}_{24} = 0.13580$ , respectively.

- (a) We seek to identify  $q_2$  with  $q_1 = \bar{q}_1$  given. The initial guess for  $q_2$  is  $q_2 \equiv 0$ ; i.e.,  $\gamma_{2m} = 0$ ,  $m = 1, \dots, 4$ .

N	$\bar{\gamma}_{21}^N$	$\bar{\gamma}_{22}^N$	$\bar{\gamma}_{23}^N$	$\bar{\gamma}_{24}^N$
2	-0.14416	0.45511	0.74438	-0.37807
4	0.13599	0.34556	0.34569	0.13577
8	0.13581	0.34569	0.34566	0.13580
16	0.13579	0.34571	0.34566	0.13580

- (b) We estimate  $q_1$  with  $q_2 = \bar{q}_2$  given (for start-up values,  $\gamma_{11} = 0.05$ ,  $\gamma_{12} = 1.5$ ,  $\gamma_{13} = 2.0$ , and  $\gamma_{14} = 2.5$  are used). The results for  $N = 3$  are given below.

$\bar{\gamma}_{11}^3$	$\bar{\gamma}_{12}^3$	$\bar{\gamma}_{13}^3$	$\bar{\gamma}_{14}^3$
0.01697	0.04321	0.04322	0.01696

#### Example 4.3

We present now our parameter estimation findings for a problem with parameters that depend on both time and space variables. We consider the system

$$\begin{cases} u_t = q_1(t, x)u_{xx} + 8(x-x^2)u_x + f(t, x), & 0 < x < 1, \quad 0 < t \leq 2 \\ u(0, x) = -20(x^2 - x) \\ u(t, 0) = u(t, 1) = 0. \end{cases}$$

A  $9 \times 3$  grid of sample data points was generated from the true solution  $\bar{u}(t, x) = -10(x^2 - x)(t^2 + 4t + 2)$ . Assuming the "true" value of  $q_1$  is given by

$\bar{q}_1(t, x) = tx$  (so that  $\bar{h}_1(t) = t$  and  $\bar{c}_1(x) = x$ ), the "true" basis coefficients for the representations of  $h_1$  in  $L^t(3)$  and  $c_1$  in  $L^x(3)$  are then given by  $\bar{\alpha}_{11} = 0$ ,  $\bar{\alpha}_{12} = \frac{2}{3}$ ,  $\bar{\alpha}_{13} = 1\frac{1}{3}$ ,  $\bar{\alpha}_{14} = 2$ , and  $\bar{\gamma}_{11} = 0$ ,  $\bar{\gamma}_{12} = \frac{1}{3}$ ,  $\bar{\gamma}_{13} = \frac{2}{3}$ ,  $\bar{\gamma}_{14} = 1$ .

Several different estimation problems were considered, using the state variable approximation index  $N = 3$  throughout.

- (a) We estimate  $h_1$  assuming  $c_1 = \bar{c}_1$  is fixed. To begin the estimation process we specify the initial guess as  $h_1(t) = 3 - \frac{3}{2}t$ ; i.e.,  $\alpha_{11} = 3$ ,  $\alpha_{12} = 2$ ,  $\alpha_{13} = 1$ , and  $\alpha_{14} = 0$ .

$\bar{\alpha}_{11}^3$	$\bar{\alpha}_{12}^3$	$\bar{\alpha}_{13}^3$	$\bar{\alpha}_{14}^3$
0.0003	0.6665	1.3338	2.0005

- (b) We wish to estimate  $c_1$  with  $h_1 = \bar{h}_1$  given. Start-up values of  $\gamma_{11} = \frac{1}{2}$ ,  $\gamma_{12} = 1$ ,  $\gamma_{13} = \frac{3}{2}$ , and  $\gamma_{14} = 2$  corresponding to an initial guess of  $c_1(x) = \frac{3}{2}x + \frac{1}{2}$  were used.

$\bar{\gamma}_{11}^3$	$\bar{\gamma}_{12}^3$	$\bar{\gamma}_{13}^3$	$\bar{\gamma}_{14}^3$
0.0061	0.3295	0.6727	0.9817

- (c) We estimate  $h_1$  and part of  $c_1$ , assuming that the first two basis coefficients of  $c_1$  are given by  $\gamma_{11} = \bar{\gamma}_{11}$  and  $\gamma_{12} = \bar{\gamma}_{12}$ . Start-up values for the remaining coefficients are  $\alpha_{11} = .5$ ,  $\alpha_{12} = .4$ ,  $\alpha_{13} = 1.8$ ,  $\alpha_{14} = 3.$ ,  $\gamma_{13} = 1.5$  and  $\gamma_{14} = 2$ .

$\bar{\alpha}_{11}^3$	$\bar{\alpha}_{12}^3$	$\bar{\alpha}_{13}^3$	$\bar{\alpha}_{14}^3$	$\bar{\gamma}_{13}^3$	$\bar{\gamma}_{14}^3$
0.0000	0.6685	1.3371	2.0054	0.6642	0.9972

Example 4.4

We conclude the section on numerical results by returning to an example similar to the dispersal model described in the introduction. To demonstrate the effectiveness of our methods for systems of this type we have chosen model equations for which the diffusion and convection coefficients are realistic from the point of view of an intended application (see the discussions in [12]). A report on our efforts to use actual field data to estimate variable diffusion, convection, and source/sink parameters in systems of the form (1.1) will appear elsewhere. Consider

$$\begin{cases} u_t + (V(t,x)u)_x = (\bar{D}u_x)_x + g(t,x), & 0 < x < 1, \quad 0 < t \leq 2, \\ u(0,x) = -400x(x-1) \\ u(t,0) = u(t,1) = 0 \end{cases}$$

where the "true" distribution of insects is given by  $\bar{u}(t,x) = -400x(x-1)\cos\frac{t}{2}$  and a constant diffusion coefficient is given by  $\bar{D} = 20$ . The time and spatially varying convection coefficient  $\bar{V}(t,x) = -100(x-.5)(4-t)$  is chosen to suggest an attraction of insects to the point  $x = .5$  (the densely vegetative center of a linear array of plants) and to indicate a decreasing attraction to the region as time increases (a reasonable model if the quantity of foodstuffs is decreasing over time). As before,  $9 \times 3$  data points are generated using  $\bar{u}$ , and the source/sink term is artificially defined to be  $g(t,x) = \bar{u}_t - (\bar{V}(t,x)\bar{u})_x - (\bar{D}\bar{u}_x)_x$ .

We remark here that although the theory developed in sections 2 and 3 (for equations in the form of (2.1)-(2.3)) may be applied to this problem with  $q_1 = \bar{D}$ ,  $q_2 = \bar{D}_x - \bar{V}$ , and  $q_3 = -\bar{V}_x$ , we cannot claim that the convergence

of  $\bar{q}_i^N(M)$  to  $\bar{q}_i(M)$ ,  $i = 1, 2$ , guarantees that  $\bar{v}^N(M) \rightarrow \bar{v}(M)$  (where  $\bar{v}^N(M) = -\bar{q}_2^N(M) + (\bar{q}_1^N(M))_x$  and  $\bar{v}(M) = -\bar{q}_2(M) + (\bar{q}_1(M))_x$ ) unless we also have the convergence of  $(\bar{q}_1^N(M))_x$  to  $(\bar{q}_1(M))_x$ . We certainly have that in the cases we consider here.

In what follows we let  $\bar{v}(t, x) = \bar{h}_2(t)\bar{c}_2(x)$  where  $\bar{h}_2(t) = 4 - t$  and  $\bar{c}_2(x) = -100(x - .5)$ . True basis coefficients for  $h_2$  as an element of  $L^t(3)$  are given by  $\bar{\alpha}_{21} = 4$ ,  $\bar{\alpha}_{22} = 3\frac{1}{3}$ ,  $\bar{\alpha}_{23} = 2\frac{2}{3}$ , and  $\bar{\alpha}_{24} = 2$ . The basis coefficients for  $\hat{P}c_2 \in S^X(1)$  (for  $\hat{P}$  the usual  $L_2$  projection of  $L_2$  onto  $S^X(1)$ ) are used for comparison as the "true" values of  $\bar{\gamma}_{2m}$ ,  $m = 1, \dots, 4$ ; those values are given by  $\bar{\gamma}_{21} = 25$ ,  $\bar{\gamma}_{22} = 8\frac{1}{3}$ ,  $\bar{\gamma}_{23} = -8\frac{1}{3}$ , and  $\bar{\gamma}_{24} = -25$ . In addition, we allow time varying estimates for  $\mathcal{D}$ , taking  $\mathcal{D} \in L^t(3)$ . "True" basis coefficients for  $\bar{\mathcal{D}} \equiv 20$  are  $\bar{\alpha}_{1k} = 20$ ,  $k = 1, \dots, 4$ . The following problems were studied and results obtained.

- (a) We estimate  $\mathcal{D}$  with  $v = \bar{v}$  given. A time-varying initial guess of  $\mathcal{D} = 40 - 15t$  (start-up values are  $\alpha_{11} = 40$ ,  $\alpha_{12} = 30$ ,  $\alpha_{13} = 20$ , and  $\alpha_{14} = 10$ ) is used.

$\bar{\alpha}_{11}^3$	$\bar{\alpha}_{12}^3$	$\bar{\alpha}_{13}^3$	$\bar{\alpha}_{14}^3$
19.9998	19.9996	19.9997	19.9997

- (b) We seek an estimate for  $h_2$ , assuming that  $c_2 = \bar{c}_2$  and  $\mathcal{D} = \bar{\mathcal{D}}$  are given. Supposing that a priori information about  $v$  indicates that it might depend on the spatial variables only, we take an initial guess of  $h_2 \equiv 1$  (or  $\alpha_{2k} = 1$ ,  $k = 1, \dots, 4$ ). The  $N = 3$  estimates for  $\alpha_{2k}$  reveal that this is indeed not the case.

$\bar{\alpha}_{21}^3$	$\bar{\alpha}_{22}^3$	$\bar{\alpha}_{23}^3$	$\bar{\alpha}_{24}^3$
4.0001	3.3335	2.6668	2.0001

- (c) We estimate  $c_2$  with  $h_2 = \bar{h}_2$  and  $D = \bar{D}$  fixed. Start-up values are  $\gamma_{2m} = 0$ ,  $m = 1, \dots, 4$ .

$\gamma_{21}^{(3)}$	$\gamma_{22}^{(3)}$	$\gamma_{23}^{(3)}$	$\gamma_{24}^{(3)}$
25.0201	8.3373	-8.3390	-24.9459

- (d) We attempt to identify  $V$  with  $D = \bar{D}$  given. Since  $V$  is the product of  $h_2$  and  $c_2$ , at least one of their basis coefficients must be fixed or there will be an infinite number of possible combinations of  $h_2$  and  $c_2$  that still yield  $h_2 c_2 = \bar{V}$ . Here we fix  $\gamma_{21} = \bar{\gamma}_{21}$  and  $\gamma_{22} = \bar{\gamma}_{22}$ . Start-up values for the remaining coefficients are  $\alpha_{2k} = 1$ ,  $k = 1, \dots, 4$ , and  $\gamma_{23} = -5$ ,  $\gamma_{24} = -15$ .

$\alpha_{21}^{(3)}$	$\alpha_{22}^{(3)}$	$\alpha_{23}^{(3)}$	$\alpha_{24}^{(3)}$	$\gamma_{23}^{(3)}$	$\gamma_{24}^{(3)}$
4.0005	3.3338	2.6670	2.0003	-8.3333	-24.9883

- (e) We repeat the calculations of (d) except that we now estimate  $\gamma_{22}$  as well (only  $\gamma_{21} = \bar{\gamma}_{21}$  is fixed in  $V$ ). Start-up values are  $\alpha_{21} = 3.2$ ,  $\alpha_{22} = 2.2$ ,  $\alpha_{23} = 1.6$ ,  $\alpha_{24} = 1.1$ ,  $\gamma_{22} = 5$ ,  $\gamma_{23} = -8.3$ , and  $\gamma_{24} = -15$ .

$\alpha_{21}^{(3)}$	$\alpha_{22}^{(3)}$	$\alpha_{23}^{(3)}$	$\alpha_{24}^{(3)}$	$\gamma_{22}^{(3)}$	$\gamma_{23}^{(3)}$	$\gamma_{24}^{(3)}$
3.7380	3.1149	2.4920	1.8689	8.9375	-8.8522	-28.6938

### §5. Concluding remarks

In the above presentation we have given a convergence theory for algorithms to estimate functional coefficients in parabolic systems. While we treated only scalar equations, the ideas generalize immediately to vector systems of equations and hence are applicable to a wide variety of transport problems in addition to the species dispersal problems that motivated our efforts here (for example, transport of several labeled substances in physiological systems such as those in the brain transport models investigated by Kyner, et.al. -- see [21], [25], [26], [2], [12], [28]). Furthermore, we believe the theoretical framework presented above is the most promising of several possible approaches in attempting to develop an estimation theory for certain nonlinear systems such as those arising in transport models with density dependent coefficients (we are currently pursuing developments in this direction) even though the framework of [7] handles some nonlinearities in a most convenient fashion.

Our basic parameter estimation ideas and techniques can also be readily extended to treat problems with several spatial variables. We have already considered theoretical aspects (with a positive outcome) and are currently developing computational packages to treat several specific problems including species dispersal in two dimensional domains and estimation in large space structures (the Maypole Hoop/Column antenna -- see [2] and [10]).

Finally, while we have not here emphasized that either boundary conditions or initial conditions or both may be unknown in many problems, such unknown parameters can easily be included in our theory and algorithms. Indeed, we have successfully used our methods to estimate boundary and initial value parameters for both parabolic and hyperbolic systems (see the discussions and results in [3], [5], [6], [7], [12]).



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